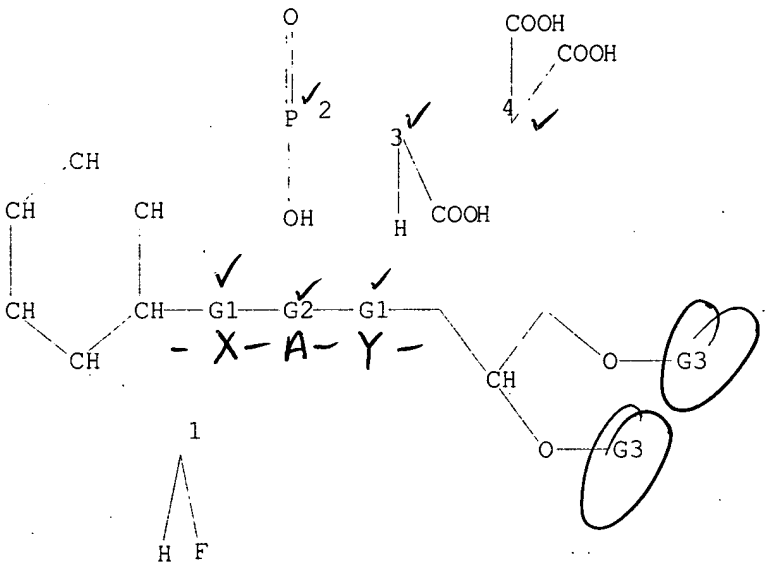
G3:Cb,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 27:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 35:CLASS 36:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,CH2,CF2,[@1]
G2 [@2],[@3],[@4]
G3 Cb,Ak

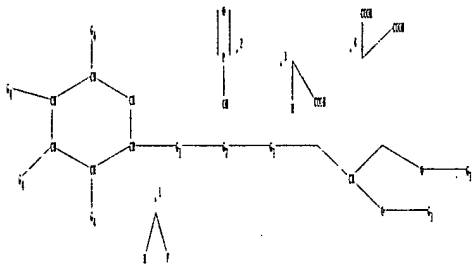
Structure attributes must be viewed using STN Express query preparation.

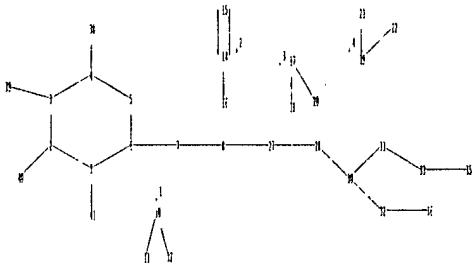
=> s l1 full
FULL SEARCH INITIATED 17:21:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 43354 TO ITERATE

100.0% PROCESSED 43354 ITERATIONS 1293 ANSWERS
SEARCH TIME: 00.00.03

L2 1293 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10526851\2.str





chain nodes :
7 8 10 11 12 14 15 16 17 18 19 20 21 22 27 28 30 31 32 33 35
36 38 39 40 41
ring nodes :
1 2 3 4 5 6
chain bonds :
1-41 2-40 3-39 4-38 6-7 7-8 8-27 10-11 10-12 14-15 14-16 17-18 17-20
19-21 19-22 27-28 28-30 30-31 30-32 31-33 32-36 33-35
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-41 2-40 3-39 4-38 5-6 6-7 7-8 8-27 27-28 30-32 31-33 32-36 33-35
exact bonds :
1-2 1-6 2-3 3-4 4-5 10-11 10-12 17-18 17-20 19-21 19-22 28-30 30-31
normalized bonds :
14-15 14-16

G1:O,CH2,CF2,[*1]

G2:[*2],[*3],[*4]

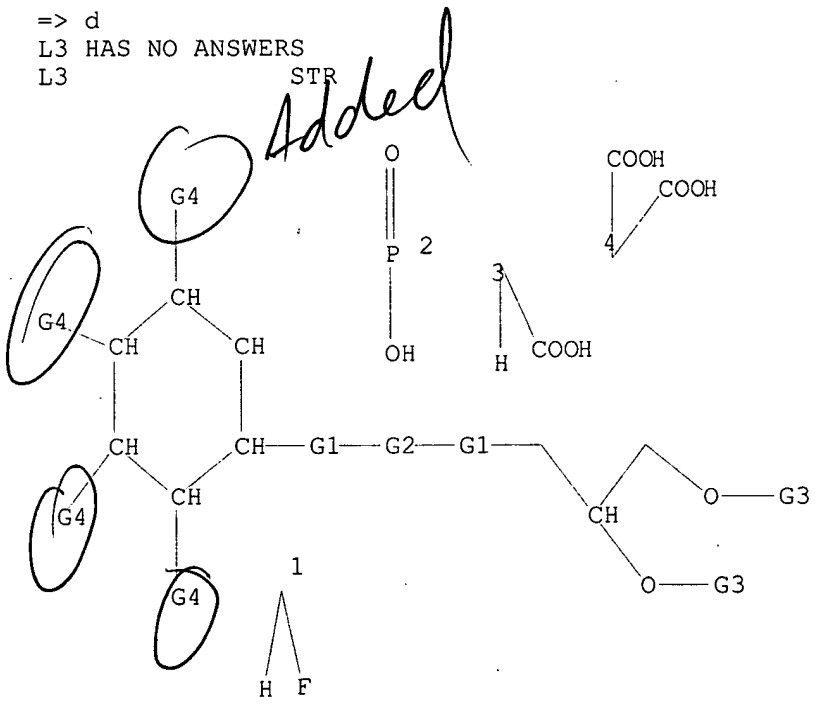
G3:Cb,Ak

G4:H,O,OH

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 27:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 35:CLASS 36:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



G1 O,CH2,CF2,[@1]

G2 [@2],[@3],[@4]

G3 Cb,Ak

G4 H,O,OH

Structure attributes must be viewed using STN Express query preparation.

=> s l3 full sub=l2
FULL SUBSET SEARCH INITIATED 17:23:40 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1293 TO ITERATE

100.0% PROCESSED 1293 ITERATIONS 1293 ANSWERS
SEARCH TIME: 00.00.01

L4 1293 SEA SUB=L2 SSS FUL L3

Same

```
=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              207.66     207.87

FILE 'CAPLUS' ENTERED AT 17:23:59 ON 14 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 14 Nov 2006  VOL 145 ISS 21
FILE LAST UPDATED: 12 Nov 2006  (20061112/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l4
L5          528 L4

=> d ibib abs hitstr 528
```

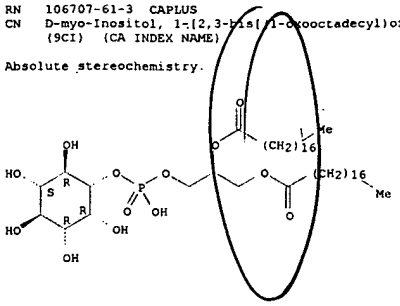
L5 ANSWER 528 OF 528 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1962:48707 CAPLUS
DOCUMENT NUMBER: 56:48707
ORIGINAL REFERENCE NO.: 56:9255e-i
TITLE: Isolation of a new lipid, triphosphoinositide, and monophosphoinositide from ox brain
AUTHOR(S): Dittmer, J. C.; Dawson, R. M. C.
CORPORATE SOURCE: Agr. Research Council Inst. Animal Physiol., Cambridge, UK
SOURCE: Biochemical Journal (1961), 81, 535-40
CODEN: BIJOAK; ISSN: 0264-6021
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 54, 22771g. A new phospholipid designated triphosphoinositide has been isolated from ox and guinea pig brains. Homogenates were extracted with CHCl3-MeOH (1:1 by volume) twice and the residue extracted 3 times with CHCl3-MeOH (2:1) containing 1 ml. concentrated HCl/400 ml. of solvent at 37°. The combined exts. were shaken with 0.2 volume of 0.9% NaCl, the interface collected, the CHCl3 solution shaken a 2nd time, and the resulting interface added to the original. The combined interracial material was shaken with a mixture of CHCl3-MeOH and NaCl of the same composition as above and the resulting interracial material collected. To this was added acetone, the mixture heated to boiling for 2 min. and dried in vacuo. The residue was treated with EtOH, evaporated to dryness in vacuo, and extracted with CHCl3-MeOH (2:1) containing 0.1 ml. concentrated HCl/200 ml. of solvent. The extract was shaken with 0.2 volume of N HCl, the mixture centrifuged, and the lower layer collected. Protein was removed by further treatment with 0.5 volume of MeOH and 0.2 volume of N HCl. The lower layer was collected, 0.5 volume MeOH added and the mixture shaken with 0.2 volume of H2O. The lower layer was collected and dried in vacuo. The crude material was dissolved in a small volume of CHCl3 (3 ml.) to which was added 20 ml. of MeOH. After 2 hrs. at -15° the precipitate formed was discarded. To the solution was slowly added at 0° methanolic NaOH (0.1N) until a pH of 6.5-7 was reached and precipitation of the Na salt was complete. The compound contained inositol, phosphate, glycerol, and fatty acid in the molar ratios of 1:3:1:2. Pretreatment of the brain tissue with acetone partially breaks the linkage in the complex, and triphosphoinositide then becomes a component of the diphosphoinositide fraction of brain tissue. Monophosphoinositide has been isolated from brain tissue and its degradation products on acid and alkaline hydrolysis indicate that it has the phosphatidyl structure (diacylglycerylphosphorylinositol).

IT 106707-61-3, Stearin, 1,2-di-, di-H phosphate, ester with inositol (from brain, structure of)

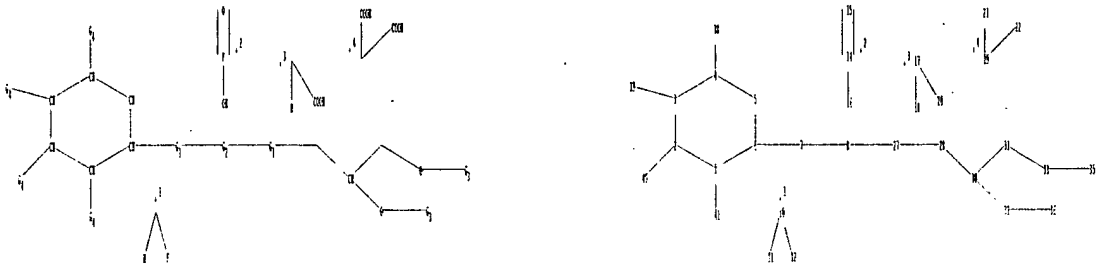
L5 ANSWER 528 OF 528 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 106707-61-3 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(1-oxooctadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



$-O-R^7 \neq \overset{O}{\overset{\|}{C}}-R^{11}$

=>
=>
Uploading C:\Program Files\Stnexp\Queries\10526851\3.str



chain nodes :
7 8 10 11 12 14 15 16 17 18 19 20 21 22 27 28 30 31 32 33 35 36 38 39 40 41
ring nodes :
1 2 3 4 5 6
chain bonds :
1-41 2-40 3-39 4-38 6-7 7-8 8-27 10-11 10-12 14-15 14-16 17-18 17-20 19-21 19-22 27-28 28-30 30-31 30-32 31-33 32-36 33-35
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-41 2-40 3-39 4-38 5-6 6-7 7-8 8-27 27-28 30-32 31-33 32-36 33-35
exact bonds :
1-2 1-6 2-3 3-4 4-5 10-11 10-12 17-18 17-20 19-21 19-22 28-30 30-31
normalized bonds :
14-15 14-16

G1:O,CH2,CF2,[*1]

G2:[*2],[*3],[*4]

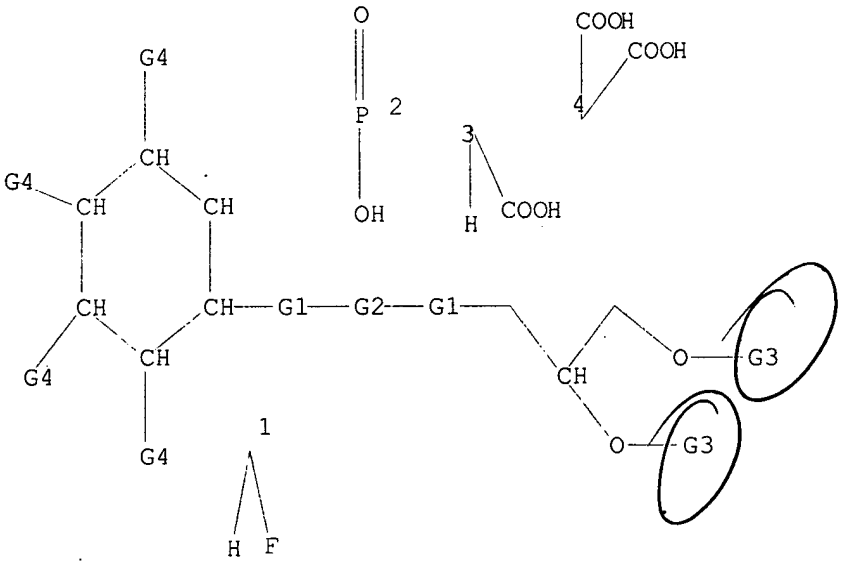
G3:Cb,CH3,CH2,CH

G4:H,O,OH

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 27:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS
33:CLASS 35:CLASS 36:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR



G1 O,CH2,CF2,[@1]

G2 [@2],[@3],[@4]

G3 Cb,Me,CH2,CH

G4 H,O,OH

Structure attributes must be viewed using STN Express query preparation.

=> s l6 full sub=L2

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 17:43:33 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1293 TO ITERATE

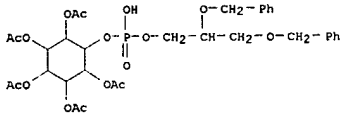
100.0% PROCESSED 1293 ITERATIONS 138 ANSWERS
SEARCH TIME: 00.00.01

L7 138 SEA SUB=L2 SSS FUL L6

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH
L8 69 L7

=> d ibib abs hitstr 69

L8 ANSWER 69 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1977:171755 CAPLUS
DOCUMENT NUMBER: 86:171755
TITLE: Synthesis of phosphatidylethanolamine and phosphatidylinositol
AUTHOR(S): Sukhanov, V. A.; Sergovskaya, N. L.; Shvets, V. I.; Estigneeva, R. P.
CORPORATE SOURCE: USSR
SOURCE: Tr. Mosk. In-ta Tonkoi Khim. Tekhnol. (1975), (6), 76-8
From: Ref. Zh., Khim. 1976, Abstr. No. 24E125
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.
IT 62700-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 62700-92-9 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentaacetate 1-[2,3-bis(phenylmethoxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 1-69

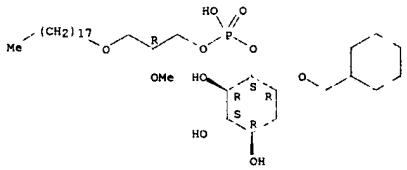
L8 ANSWER 1 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:239690 CAPLUS
DOCUMENT NUMBER: 145:477
TITLE: Spectrum of activity and molecular correlates of response to phosphatidylinositol ether lipid analogues, novel lipid-based inhibitors of Akt
AUTHOR(S): Gills, Joell J.; Holbeck, Susan; Hollingshead, Melinda; Hewitt, Stephen M.; Kozikowski, Alan P.; Dennis, Phillip A.
CORPORATE SOURCE: Medical Oncology Branch and Tissue Array Research Program, Laboratory of Pathology, Center for Cancer Research, National Cancer Institute, Bethesda, MD, USA
SOURCE: Molecular Cancer Therapeutics (2006), 5(3), 713-722
CODEN: MCTOCF; ISSN: 1535-7163
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The serine/threonine kinase Akt is a promising target in cancer. We previously identified five phosphatidylinositol ether lipid analogs (PIA) that inhibited Akt activation and selectively killed lung and breast cancer cells with high levels of Akt activity. To assess the spectrum of activity in other cell types and to compare PIAs with other inhibitors of the phosphatidylinositol 3-kinase (PI3K)/Akt/mammalian target of rapamycin (mTOR) pathway, we compared growth inhibition by PIAs against the PI3K inhibitors LY294002 and wortmannin and the mTOR inhibitor rapamycin in the NCI60 cell line panel. Although each of these compds. inhibited the growth of all the cell lines, distinct patterns were observed The PIAs were the least potent but the most cytotoxic. The broad spectrum of activity of PIAs was confirmed in vivo in hollow fiber assays. The response to PIAs was significantly correlated with levels of active but not total Akt in the NCI60, as assessed using COMPARE anal. However, a number of mol. targets were identified whose expression was more highly correlated with sensitivity to PIAs than active Akt. Expression of these mol. targets did not overlap with those that correlated with sensitivity to LY294002, wortmannin, or rapamycin. A COMPARE anal. of the National Cancer Institute chemical screening database revealed that the patterns of activity of PIAs correlated best with patterns of activity of other lipid-based compds. These studies show that although PIAs are widely active in cancer cells, which correlates with the presence of its intended target, active Akt, PIAs are biol. distinct from other known inhibitors of the PI3K/Akt/mTOR pathway.

IT 701976-54-7 701976-55-8 701976-68-3
701976-69-4 701976-70-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phosphatidylinositol ether lipid analogs as inhibitors of Akt in cancer)

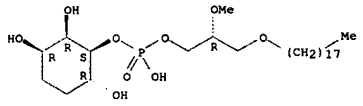
RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-

L8 ANSWER 1 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 701976-70-7 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1S,2R,3R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

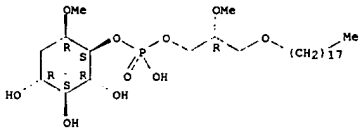
Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

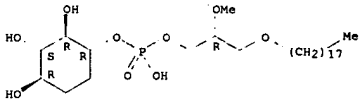
L8 ANSWER 1 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



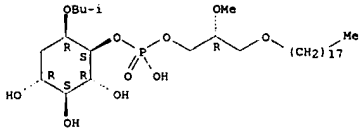
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-68-3 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-(2-methylpropyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-69-4 CAPLUS
CN L-chiro-Inositol, 1-O-(cyclohexylmethyl)-6-deoxy-, 2-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 2 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:167377 CAPLUS
DOCUMENT NUMBER: 144:249992
TITLE: Self-renewal and differentiation in human embryonic stem cells in the presence of PI3-kinase pathway inhibitor and TGFβ family member
INVENTOR(S): Dalton, Stephen; Sheppard, Allan; Jones, Karen; Baetge, E. Edward; D'Amour, Kevin A.; Agulnick, Alan D.
PATENT ASSIGNEE(S): University of Georgia Research Foundation, Inc., USA; Cythera, Inc.
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006020919	A2	20060223	WO 2005-US28829	20050815

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-601664P P 20040813

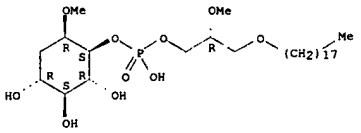
AB The present invention provides compns. and methods for the production of differentiated mammalian cells (e.g., human cells). More particularly, the present invention provides cellular differentiation methods employing culturing the cells on a feeder layer or under feeder-free conditions in cell culture and further contacting the cells with an inhibitor of the PI3-kinase pathway (e.g., rapamycin) and a member of the TGFβ family (e.g., activin A) for the generation of differentiated mammalian cells from pluripotent mammalian stem cells. The differentiated cell is selected from the group consisting of a mesendodermal cell, a mesodermal cell, and an endodermal cell (preferably, an endodermal cell).

IT 701976-54-7, Akt inhibitor II
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(PI3 inhibitor SH5; self-renewal and differentiation in human embryonic stem cells in presence of PI3-kinase pathway inhibitor and TGFβ family member)

RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

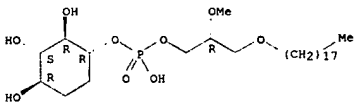
Absolute stereochemistry.

L8 ANSWER 2 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

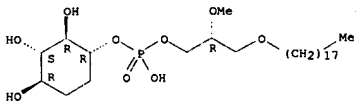


IT 701976-55-8, Akt inhibitor III
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(PI3 inhibitor SH6; self-renewal and differentiation in human embryonic
stem cells in presence of PI3-kinase pathway inhibitor and TGFβ family member)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:65453 CAPLUS
DOCUMENT NUMBER: 145:305797
TITLE: Bcl-2 attenuates anticancer agents-induced apoptosis by sustained activation of Akt/protein kinase B in U937 cells
AUTHOR(S): Woo, K. J.; Yoo, Y. H.; Park, J.-W.; Kwon, T. K.
CORPORATE SOURCE: Department of Immunology, School of Medicine, Keimyung
University, Taegu, 700-712, S. Korea
SOURCE: Apoptosis (2005), 10(6), 1333-1343
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Aberrant overexpression of antiapoptotic members of the Bcl-2 protein family contributes to resistance to anticancer therapeutic drugs. Thus, this protein represent attractive target for novel anticancer agents. In the present study, we determined the effect of the anti-apoptosis protein Bcl-2
on caspase-3 activation, PLC-γ1 degradation and Akt activation during the various anticancer agents-induced apoptosis. Treatment with chrysin for 12 h produced morphol. features of apoptosis in U937 cells, which was associated with caspase-3 activation and PLC-γ1 degradation Induction of
apoptosis was also accompanied by down-regulation of XIAP and inactivation
of Akt. Chrysin-induced caspase-3 activation, PLC-γ1 degradation and apoptosis were significantly attenuated in Bcl-2 overexpressing U937/Bcl-2
cells. Ectopic expression of Bcl-2 appeared to inhibit ceramide-, and Akt
specific inhibitor (SH-6)-induced apoptosis by sustained Akt activation. Thus, our findings imply that some of the biol. functions of Bcl-2 may be attributed to their ability to inhibit anticancer agents-induced apoptosis
through the sustained Akt activation.
IT 701976-55-8, SH 6 (enzyme inhibitor)
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(induction of apoptosis was also accompanied by down-regulation of XIAP
and inactivation of Akt)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 4 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:984081 CAPLUS
DOCUMENT NUMBER: 143:300314
TITLE: Sequences of novel human APO2L and IL-24 splice variant polypeptides, polynucleotides, and methods of their use in cancer therapy
INVENTOR(S): Wang, Yan; Collins, Amy L. Tsui; Hestir, Kevin; Lee, Ernestine; Halenbeck, Robert Forgan; Bosch, Elizabeth;
Linnemann, Thomas; Williams, Lewis T.
PATENT ASSIGNEE(S): Five Prime Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082934	A2	20050909	WO 2005-US5221	20050218
WO 2005082934	A3	20051215		

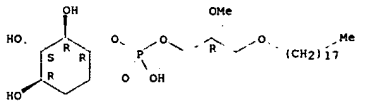
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:		
US 2004-546385P	P	20040220
US 2005-647013P	P	20050127
US 2005-654229P	P	20050218

AB The present invention discloses newly identified human interleukin 24 and APO2L splice variant mols., their polypeptide sequences, and the polynucleotides encoding the polypeptide sequences. Also provided is a procedure for producing such polypeptides by recombinant techniques employing, for example, vectors and host cells, and, for example, heterologous secretory leader sequences. Also disclosed are methods for using such polypeptides and modulators thereof for the treatment of diseases, including cancer, immune diseases, infectious diseases, and ischemic diseases.
IT 701976-55-8, SH 6
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sequences of novel human APO2L and IL-24 splice variant polypeptides, polynucleotides, and methods of their use in cancer therapy)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 4 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L8 ANSWER 5 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:451176 CAPLUS
DOCUMENT NUMBER: 143:1222
TITLE: Modulating substances of the nitric oxide-cyclic guanosine 3',5'-monophosphate signaling pathway for the treatment of dental disorders
INVENTOR(S): Baumann, Michael; Bloch, Wilhelm; Korkmaz, Yueksel
PATENT ASSIGNEE(S): Cell Center Cologne G.m.b.H., Germany
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005046660	A1	20050526	WO 2004-EP12935	20041115

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 2003-26132 A 20031113

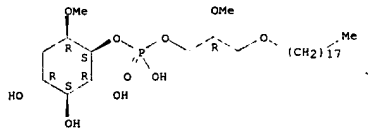
AB The use of a modulating substance of the nitric oxide (NO)-cyclic guanosine 3',5'-monophosphate (cGMP) signaling pathway for the preparation of a pharmaceutical composition for the prevention and/or treatment of a dental disorder in a mammal is disclosed. Furthermore, pharmaceutical compns. comprising a modulating substance of the NO-cGMP signaling pathway as well as methods for treating a dental disorder are provided.

IT 701976-54-7, SH 5 701976-55-8, SH 6
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(modulating substances of the nitric oxide-cyclic GMP signaling pathway for the treatment of dental disorders)

RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

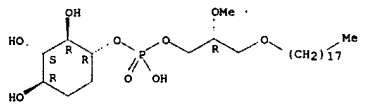
Absolute stereochemistry.

L8 ANSWER 5 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:339752 CAPLUS
DOCUMENT NUMBER: 143:109462
TITLE: Fenofibrate induces apoptotic injury in cultured human hepatocytes by inhibiting phosphorylation of Akt
AUTHOR(S): Kubota, T.; Yano, T.; Fujisaki, K.; Itoh, Y.; Oishi, R.
CORPORATE SOURCE: Department of Pharmacy, Kyushu University Hospital, Higashi-ku, Fukuoka, 812-8582, Japan
SOURCE: Apoptosis (2005), 10(2), 349-358
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

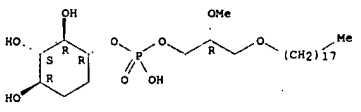
AB Fibric acid derivs. have a potent and effective lipid-lowering action, however, the use of these compds. is sometimes limited due to the occurrence of hepatic injury. In the present study, we characterized cell injury induced by fenofibrate in cultured human hepatocytes. Fenofibrate caused a loss of cell viability and nuclear damage as assessed by terminal deoxynucleotidyl transferase-mediated dUTP nick end-labeling or by DNA electrophoresis, in which caspase activation is involved. The cell injury was accompanied by the shrinkage and the translocation of phosphatidyl serine from inner membrane to the outer membrane as determined by annexin V stain. The mRNA expression for bcl-2 was reduced by fenofibrate. An immunofluorescent stain with antiserum raised against phosphorylated Akt revealed that fenofibrate inhibited insulin-stimulated phosphorylation of Akt. Like fenofibrate, several compds. that inhibit the phosphorylation of Akt, including wortmannin, SH-6 and a high concentration (100 μM) of SB203580, reduced the viability of cultured human hepatocytes. Both nuclear damage and cell injury induced by fenofibrate were reversed by insulin in a concentration-dependent manner. In contrast, bezafibrate or 8(S)-hydroxyeicosatetraenoic acid had no hepatotoxic action. These findings suggest that fenofibrate causes caspase-dependent apoptosis in human hepatocytes by inhibiting phosphorylation of Akt, in which PPARα is not involved.

IT 701976-55-8
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(fenofibrate caused caspase-dependent apoptosis in human hepatocytes by inhibiting phosphorylation of Akt, in which peroxisome proliferator-activated receptor-α was not involved)

RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 6 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 7 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:141521 CAPLUS
DOCUMENT NUMBER: 142:423232
TITLE: TRAIL-induced apoptosis in gliomas is enhanced by Akt-inhibition and is independent of JNK activation
AUTHOR(S): Puduvalli, V. K.; Sampath, D.; Bruner, J. M.; Nangia, J.; Xu, R.; Kyritsis, A. P.
CORPORATE SOURCE: Departments of Neuro-Oncology, The University of Texas M. D. Anderson Cancer Center, Houston, TX, 77030, USA
SOURCE: Apoptosis (2005), 10(1), 233-243
CODEN: APOPFN; ISSN: 1360-8185
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

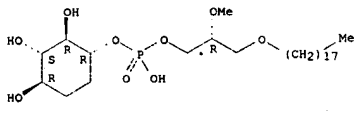
AB Patients with malignant gliomas have a poor prognosis and new treatment paradigms are needed against this disease. TRAIL/Apo2L selectively induces apoptosis in malignant cells sparing normal cells and is hence of interest as a potential therapeutic agent against gliomas. To determine the factors that modulate sensitivity to TRAIL, we examined the differences in TRAIL-activated signaling pathways in glioma cells with variable sensitivities to the agent. Apoptosis in response to TRAIL was unrelated to DR5 expression or endogenous p53 status in a panel of 8 glioma cell lines. TRAIL activated the extrinsic (cleavage of caspase-8, caspase-3 and PARP) and mitochondrial apoptotic pathways and reduced FLIP levels. It also induced caspase-dependent JNK activation, which did not influence TRAIL-induced apoptosis. Because the pro-survival PI3K/Akt pathway is highly relevant to gliomas, we assessed whether Akt could protect against TRAIL-induced apoptosis. Pretreatment with SH-6, a novel Akt inhibitor, enhanced TRAIL-induced apoptosis, suggesting a protective role for Akt. Conversely, TRAIL induced caspase-dependent cleavage of Akt neutralizing its anti-apoptotic effects. These results demonstrate that TRAIL-induced apoptosis in gliomas involves both activation of death pathways and downregulation of survival pathways. Addnl. studies are warranted to determine the therapeutic potential of TRAIL against gliomas.

IT 701976-55-8, SH 6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Akt inhibitor SH-6 enhanced TNF-related apoptosis inducing ligand induced apoptosis in human malignant glioma D54MG, U251MG, U87MG, U343, U373, A172, LN229, T98G cells)

RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 7 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

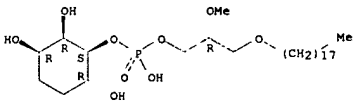
L8 ANSWER 8 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:133799 CAPLUS
DOCUMENT NUMBER: 142:423229
TITLE: Activated forms of H-RAS and K-RAS differentially regulate membrane association of PI3K, PDK-1, and AKT and the effect of therapeutic kinase inhibitors on cell survival
AUTHOR(S): Caron, Ruben W.; Yacoub, Adly; Li, Min; Zhu, Xiaoyu; Mitchell, Clint; Hong, Young; Hawkins, William; Sasazuki, Takehiko; Shirasawa, Senji; Kozikowski, Alan P.; Dennis, Philip A.; Hagan, Michael P.; Grant, Steven; Dent, Paul
CORPORATE SOURCE: Departments of Radiation Oncology and Hematology/Oncology, Virginia Commonwealth University, Richmond, VA, USA
SOURCE: Molecular Cancer Therapeutics (2005), 4(2), 257-270
CODEN: MCTOCF; ISSN: 1535-7163
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The abilities of mutated active RAS proteins to modulate cell survival following exposure to ionizing radiation and small mol. kinase inhibitors were examined Homologous recombination in HCT116 cells to delete the single allele of K-RAS D13 resulted in a cell line that exhibited an .apprx.75% reduction in basal extracellular signal-regulated kinase 1/2, AKT, and c-jun-NH2-kinase 1/2 activity. Transfection of cells lacking K-RAS D13 with H-RAS V12 restored extracellular signal-regulated kinase 1/2 and AKT activity to basal levels but did not restore c-jun-NH2-kinase 1/2 phosphorylation. In cells expressing H-RAS V12, radiation caused prolonged intense activation of AKT. Inhibition of H-RAS V12 function, blockade of phosphatidylinositol 3-kinase (PI3K) function using small interfering RNA/small-mol. inhibitors, or expression of dominant-neg. AKT abolished radiation-induced AKT activation, and radiosensitized these cells. Inhibition of PI3K function did not significantly radiosensitize parental HCT116 cells. Inhibitors of the AKT PH domain including perifosine, SH-(5, 23 - 25) and ml-(14 - 16) reduced the plating efficiency of H-RAS V12 cells in a dose-dependent fashion. Inhibition of AKT function using perifosine enhanced radiosensitivity in H-RAS V12 cells, whereas the SH and ml series of AKT PH domain inhibitors failed to promote radiation toxicity. In HCT116 H-RAS V12 cells, PI3K, PDK-1, and AKT were membrane associated, whereas in parental cells expressing K-RAS D13, only PDK-1 was membrane bound. In H-RAS V12 cells, membrane associated PDK-1 was phosphorylated at Y373/376, which was abolished by the Src family kinase inhibitor PP2. Inhibition of PDK-1 function using the PH domain inhibitor OSU-03012 or using PP2 reduced the plating efficiency of H-RAS V12 cells and profoundly increased radiosensitivity. OSU-03012 and PP2 did not radiosensitize and had modest inhibitory effects on plating efficiency in parental cells. A small interfering RNA generated against PDK1 also radiosensitized HCT116 cells expressing H-RAS V12. Collectively, our data argue that mol. inhibition of AKT and PDK-1 signaling enhances the radiosensitivity of HCT116 cells expressing H-RAS V12 but not K-RAS D13. Small-mol. inhibitory agents that blocked stimulated and/or basal PDK-1 and AKT function profoundly reduced HCT116 cell survival but had variable effects at enhancing tumor cell radiosensitivity.

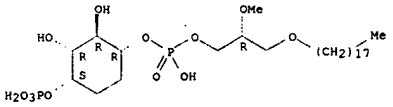
L8 ANSWER 8 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
IT 701976-70-7 850894-86-9 850894-87-0
850894-89-2 850894-90-5 850894-91-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(activated forms of H-RAS and K-RAS differentially regulate membrane association of PI3K, PDK-1, and AKT and the effect of therapeutic kinase
inhibitors on cell survival)
RN 701976-70-7 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1S,2R,3R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



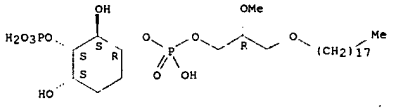
RN 850894-86-9 CAPLUS
CN Phosphoric acid, mono[(1R,2R,3R,4S)-2,3-dihydroxy-4-(phosphonooxy)cyclohexyl] mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850894-87-0 CAPLUS
CN Phosphoric acid, mono[(1R,2S,3S,4S)-2,4-dihydroxy-3-(phosphonooxy)cyclohexyl] mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

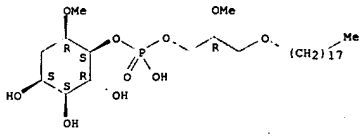


L8 ANSWER 8 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

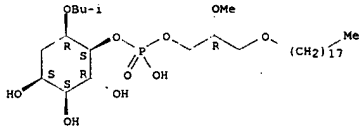
RN 850894-89-2 CAPLUS
CN D-epi-Inositol, 3-deoxy-2-O-methyl-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



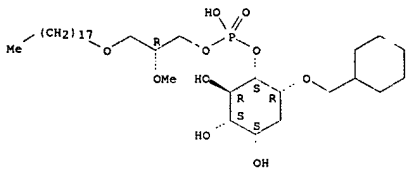
RN 850894-90-5 CAPLUS
CN D-epi-Inositol, 3-deoxy-2-O-(2-methylpropyl)-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 850894-91-6 CAPLUS
CN D-epi-Inositol, 2-O-(cyclohexylmethyl)-3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

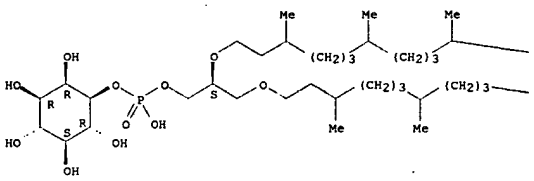


L8 ANSWER 9 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1103060 CAPLUS
DOCUMENT NUMBER: 142:194102
TITLE: Cold adaptation in the Antarctic archaeon Methanococcoides burtonii involves membrane lipid unsaturation
AUTHOR(S): Nichols, David S.; Miller, Matthew R.; Davies, Noel W.; Goodchild, Amber; Raftery, Mark; Cavicchioli, Ricardo
CORPORATE SOURCE: Australian Food Safety Centre of Excellence, University of Tasmania, Tasmania, Australia
SOURCE: Journal of Bacteriology (2004), 186(24), 8508-8515
CODEN: JOBAAY; ISSN: 0021-9193
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Direct anal. of membrane lipids by liquid chromatog.-electrospray mass spectrometry was used to demonstrate the role of unsatn. in ether lipids in the adaptation of Methanococcoides burtonii to low temperature A proteomics
approach using two-dimensional liquid chromatog.-mass spectrometry was used
to identify enzymes involved in lipid biosynthesis, and a pathway for lipid biosynthesis was reconstructed from the M. burtonii draft genome sequence. The major phospholipids were archaeol phosphatidylglycerol, archaeol phosphatidylinositol, hydroxyarchaeol phosphatidylglycerol, and hydroxyarchaeol phosphatidylinositol. All phospholipid classes contained a series of unsatd. analogs, with the degree of unsatn. dependent on phospholipid class. The proportion of unsatd. lipids from cells grown at 4°C was significantly higher than for cells grown at 23°C. 3-Hydroxy-3-methylglutaryl CoA synthase, farnesyl diphosphate synthase, and geranylgeranyl diphosphate synthase were identified in the expressed proteome, and most genes involved in the mevalonate pathway and processes leading to the formation of phosphatidylinositol and phosphatidylglycerol were identified in the genome sequence. In addition, M. burtonii encodes CDP-inositol and CDP-glycerol transferases and a number of homologs of the
plant geranylgeranyl reductase. It therefore appears that the unsatn. of lipids may be due to incomplete reduction of an archaeol precursor rather than
to a desaturase mechanism. This study shows that cold adaptation in M. burtonii involves specific changes in membrane lipid unsatn. It also demonstrates that global methods of anal. for lipids and proteomics linked
to a draft genome sequence can be effectively combined to infer specific mechanisms of key biol. processes..
IT 839727-90-1 839727-91-2
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(cold adaptation in Antarctic archaeon Methanococcoides burtonii involves membrane lipid unsatn.)
RN 839727-90-1 CAPLUS
CN D-myo-Inositol,
1-[(2S)-2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

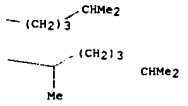
Absolute stereochemistry.
Currently available stereo shown.

L8 ANSWER 9 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



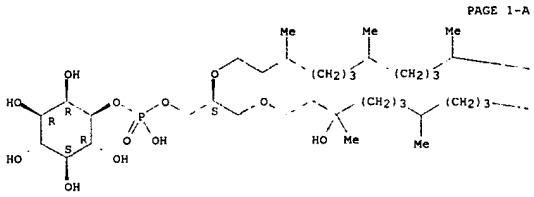
PAGE 1-B



RN 839727-91-2 CAPLUS
CN D-myo-Inositol,
1-[(2S)-3-[(3-hydroxy-3,7,11,15-tetramethylhexadecyl)oxy]-
2-[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI)
(CA INDEX NAME)

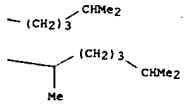
Absolute stereochemistry.
Currently available stereo shown.

PAGE 1-A



L8 ANSWER 9 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

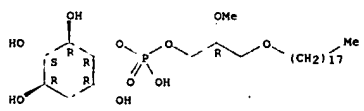
PAGE 1-B



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 10 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1087440 CAPLUS
DOCUMENT NUMBER: 142:273578
TITLE: In vivo molecular pharmacology and antitumor activity of the targeted Akt inhibitor PX-316
AUTHOR(S): Meuillet, Emmanuelle J.; Ihle, Nathan; Baker, Amanda F.; Gard, Jaime M.; Stamper, Chelsea; Williams, Ryan; Coon, Amy; Mahadevan, Daruka; George, Benjamin L.; Kirkpatrick, Lynn; Powis, Garth
CORPORATE SOURCE: Arizona Cancer Center, University of Arizona, Tucson, AZ, 85724, USA
SOURCE: Oncology Research (2004), 14(10), 513-527
CODEN: ONREE8; ISSN: 0965-0407
PUBLISHER: Cognizant Communication Corp.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Akt, a serine/threonine kinase that promotes cell survival, is activated by binding of its pleckstrin homol. (PH) domain to membrane phosphatidylinositol (PtdIns)-3-phosphates formed by PtdIns-3-kinase. D-3-Deoxy-phosphatidyl-myo-inositols that cannot be phosphorylated on the 3-position of the myo-inositol group are inhibitors of the Akt PH domain. The most active compound is D-3-deoxy-phosphatidyl-myo-inositol 1-[(R)-2-methoxy-3-octadecyloxypropyl hydrogen phosphate] (PX-316). PX-316 administered i.p. to mice at 150 mg/kg inhibits Akt activation in HT-29 human tumor xengrafts up to 78% at 10 h with recovery to 34% at 48 h. Phosphorylation of GSK-3β, a downstream target of Akt, is also inhibited. There is no decrease in PtdIns(3,4,5)-trisphosphate levels by PX-316, showing it is not an inhibitor of PtdIns-3-K in vivo. Gene expression profiling of HT-29 tumor xenografts shows many similarities between the effects of PX-316 and the PtdIns-3-K inhibitor wortmannin, with downregulation of several ribosomal-related genes, while PX-316 uniquely increases the expression of a group of mitochondrial-related genes. PX-316 has antitumor activity against early human MCF-7 breast cancer and HT-29 colon cancer xenografts in mice. PX-316 formulated in 20% hydroxypropyl-β-cyclodextrin for i.v. administration is well tolerated in mice and rats with no hemolysis and no hematol. toxicity. Thus, PX-316 is the lead compound of a new class of potential agents that inhibit Akt survival signaling.
IT 253440-95-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Akt inhibitor PX-316 inhibited phosphorylation of its downstream targets in human HT-29 tumor xenograft in SCID mouse without inhibiting
(ptdIns2)-3-K, showed antitumor activity on human MCF-7, HT-29 xenograft and less toxic in rat, mouse)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 10 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

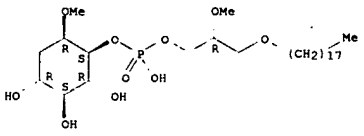
L8 ANSWER 11 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:759995 CAPLUS
DOCUMENT NUMBER: 142:126804
TITLE: Novel 2'-substituted, 3'-deoxy-phosphatidyl-myo-inositol analogues reduce drug resistance in human leukaemia cell lines with an activated phosphoinositide 3-kinase/Akt pathway
AUTHOR(S): Tabellini, Giovanna; Tazzari, Pier Luigi; Bortul, Roberta; Billi, Anna Maria; Conte, Roberto; Manzoli, Lucia; Cocco, Lucio; Martelli, Alberto M.
CORPORATE SOURCE: Dipartimento di Scienze Anatomiche Umane e Fisiopatologia dell'Apparato Locomotore, Sezione di Anatomia, Cell Signaling Laboratory, Universita di Bologna, Bologna, Italy
SOURCE: British Journal of Haematology (2004), 126(4), 574-582
CODEN: BJHEAL; ISSN: 0007-1048
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Activation of the phosphoinositide 3-kinase (PI3-K)/Akt signalling pathway has been linked with resistance to chemotherapeutic drugs, and its down-regulation, by means of pharmacol. inhibitors of PI3-K, considerably lowers resistance to various types of therapy in cell lines derived from solid tumors. Recently, a new class of Akt inhibitors, referred to as phosphatidylinositol ether lipids (PIAs), have been synthesized. We tested whether two new PIAs could lower the sensitivity threshold to chemotherapeutic drugs of human leukemia cell lines with an activated PI3-K/Akt network. We used HL60AR (for apoptosis resistant), K562 and U937 cells. The two pharmacol. inhibitors, used at 5 μmol/l, down-regulated Akt kinase activity and phosphorylation. Neither of the two chems. affected the activity of other signalling proteins in the Akt pathway, such as phosphoinositide-dependent protein kinase-1 or PTEN. When employed at 5 μmol/l, the Akt inhibitors markedly reduced the resistance of the leukemic cell lines to etoposide or cytarabine. Remarkably, a 5 μmol/l concentration of the inhibitors did not neg. affect the survival rate of human cord blood CD34+ cells. Overall, our results indicate that new selective Akt pharmacol. inhibitors might be used in the future for overcoming Akt-mediated resistance to therapeutic treatments of acute leukemia cells.

IT 701976-54-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(SH-5; Akt inhibitors SH-5 and SH-6 decreased Akt kinase activity, phosphorylation, reduced leukemic cell resistance to etoposide and cytarabine but gave no effect on PTEN and CB CD34+ survival rate in HL60AR, HL60PT, K562 and U937 cell line)
RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

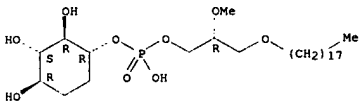
Absolute stereochemistry.

L8 ANSWER 11 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 701976-55-8, D-2,3-Dideoxy-2-myo-inositol 1-[(R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate]
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(SH-6; Akt inhibitors SH-5 and SH-6 decreased Akt kinase activity, phosphorylation, reduced leukemic cell resistance to etoposide and cytarabine but gave no effect on PTEN and CB CD34+ survival rate in HL60AR, HL60PT, K562 and U937 cell line)
RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:610046 CAPLUS
DOCUMENT NUMBER: 141:150985
TITLE: Antineoplastic ether lipid compounds
INVENTOR(S): Perkins, Walter R.
PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

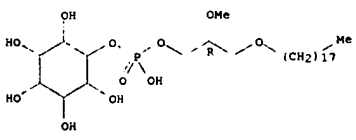
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004062586	A2	20040729	WO 2004-US267	20040108
WO 2004062586	A3	20041209		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ				
EP 1583552	A2	20051012	EP 2004-700830	20040108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006135765	A1	20060622	US 2005-541863	20051110
PRIORITY APPLN. INFO.:			US 2003-438786P	P 20030109
			WO 2004-US267	W 20040108

OTHER SOURCE(S): MARPAT 141:150985

AB Ether lipid compds. and pharmaceutically-acceptable salts, prodrugs or isomers thereof are described. The compds. of the invention have antineoplastic activity, and accordingly have utility in treating cancer and related diseases. Enantiomers of these compds., pharmaceutical compns., and methods for treating cancer with the pharmaceutical compns. are also provided. For example, preparation and screening of 2'-trimethylaminoethyl-1-O-octadecyl-2-O-methylbutane-4-phosphonate was presented.

IT 728881-95-6P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ether lipid compds. for cancer treatment)
RN 728881-95-6 CAPLUS
CN Inositol, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 12 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L8 ANSWER 13 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:412760 CAPLUS
DOCUMENT NUMBER: 140:417918
TITLE: Hydroxyflutamide induced pathways related to androgen receptor negative prostate cancer cells
INVENTOR(S): Chang, Chawnshang; Lee, Yi-fen; Lin, Wen-jye
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041185	A2	20040521	WO 2003-US34636	20031031
WO 2004041185	A3	20040826		

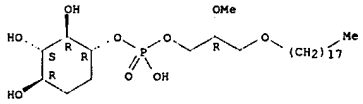
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003287366	A1	20040607	AU 2003-287366	20031031
PRIORITY APPLN. INFO.:			US 2002-423340P	P 20021031
			WO 2003-US34636	W 20031031

AB Disclosed are compns. and methods for reducing androgen receptor dependent cancer cell proliferation. To overcome the problems associated with androgen ablation treatment and more specifically antiandrogen withdrawal syndrome, disclosed herein are compns. comprising combination therapies for the treatment of prostate cancer based on the links in prostate cancer and the pathways disclosed herein. Thus disclosed are compns. comprising an inhibitor of the MAP kinase or MEK pathway signal transduction pathway and an antiandrogen, such as flutamide or hydroxyflutamide. Also, specifically disclosed are compns. comprising an antiandrogen and an anti-phosphatidylinositol 3-kinase (PI3K)/Akt kinase inhibitor.
IT 701976-55-8, SH 6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hydroxyflutamide induced pathways related to androgen receptor neg. prostate cancer cells in relation to treatment with antiandrogens and kinase pathway inhibitors and drug screening)
RN 701976-55-8 CAPLUS

L8 ANSWER 13 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

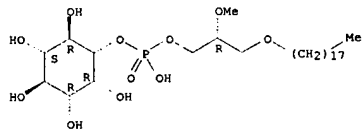


10/31/03
10/31/02 X

L8 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:309668 CAPLUS
DOCUMENT NUMBER: 141:33428
TITLE: Preferential Inhibition of Akt and Killing of Akt-Dependent Cancer Cells by Rationally Designed Phosphatidylinositol Ether Lipid Analogues
AUTHOR(S): Castillo, S. Sianna; Brognard, John; Petukhov, Pavel A.; Zhang, Chunyu; Tsurutani, Junji; Granville, Courtney A.; Li, Min; Jung, Michael; West, Kip A.; Gills, Joell G.; Kozikowski, Alan P.; Dennis, Phillip A.
CORPORATE SOURCE: Center for Cancer Research, Cancer Therapeutics Branch, National Cancer Institute, Bethesda, MD, USA
SOURCE: Cancer Research (2004), 64(8), 2782-2792
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Activation of the PI3k/Akt pathway controls key cellular processes and contributes to tumorigenesis in vivo, but investigation of the PI3k/Akt pathway has been limited by the lack of specific inhibitors directed against Akt. To develop Akt inhibitors, we used mol. modeling of the pleckstrin homol. (PH) domain of Akt to guide synthesis of structurally modified phosphatidylinositol ether lipid analogs (PIAs). Here, we characterize the biochem. and cellular effects of PIAs. Of 24 compds. tested, five PIAs with modifications at two sites on the inositol ring inhibited Akt with IC50s < 5 μM. Mol. modeling identified putative interactions of PIAs with the phosphoinositide-binding site in the PH domain of Akt, and growth factor-induced translocation of Akt to the plasma membrane was inhibited by PIA administration. Inhibition of Akt occurred rapidly and was maintained for hours. PIAs decreased phosphorylation of many downstream targets of Akt without affecting upstream kinases, such as PI3k or phosphoinositide-dependent kinase-1, or members of other kinase pathways such as extracellular signal-regulated kinase. Importantly, PIAs increased apoptosis 20 - 30-fold in cancer cell lines with high levels of endogenous Akt activity but only 4 ~ 5-fold in cancer cell lines with low levels of Akt activity. These studies identify PIAs as effective Akt inhibitors, and provide proof of principle for targeting the PH domain of Akt.
IT 213408-29-8 701976-54-7 701976-55-8 701976-57-0 701976-59-2 701976-62-7 701976-65-0 701976-67-2 701976-68-3 701976-69-4 701976-70-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preferential inhibition of Akt and killing of Akt-dependent cancer cells by rationally designed phosphatidylinositol ether lipid analogs)
RN 213408-29-8 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2-methoxy-1-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

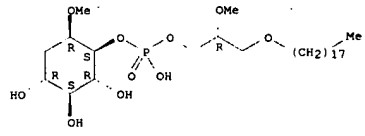
Absolute stereochemistry.

L8 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



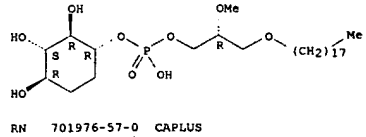
RN 701976-54-7 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-methyl-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-55-8 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

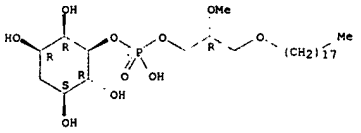
Absolute stereochemistry.



RN 701976-57-0 CAPLUS
CN D-epi-Inositol, 4-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

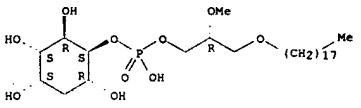
Absolute stereochemistry.

L8 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



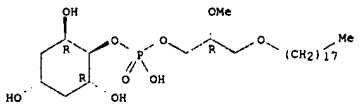
RN 701976-59-2 CAPLUS
CN D-allo-Inositol, 2-deoxy-, 6-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-62-7 CAPLUS
CN Phosphoric acid, mono[2-methoxy-3-(octadecyloxy)propyl] mono[(1α,2R,4β,6R)-2,4,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



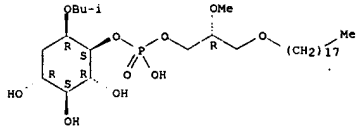
RN 701976-65-0 CAPLUS
CN Phosphoric acid, P,P'-[1,6-hexanediylbis[oxy[(2R)-2-methoxy-3,1-propanediyl]]] P,P'-bis[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

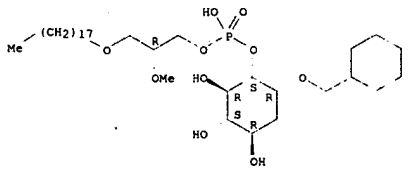
RN 701976-68-3 CAPLUS
CN L-chiro-Inositol, 1-deoxy-6-O-(2-methylpropyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



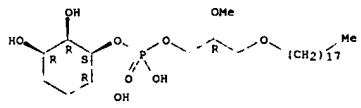
RN 701976-69-4 CAPLUS
CN L-chiro-Inositol, 1-O-(cyclohexylmethyl)-6-deoxy-, 2-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 701976-70-7 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1S,2R,3R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

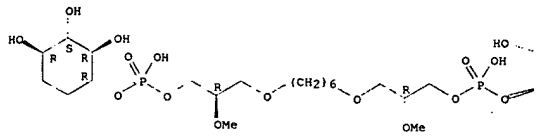
Absolute stereochemistry.



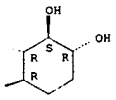
REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



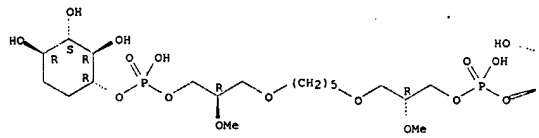
PAGE 1-B



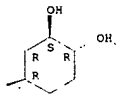
RN 701976-67-2 CAPLUS
CN Phosphoric acid, P,P'-[1,5-pentanediylbis[oxy[(2R)-2-methoxy-3,1-propanediyl]]] P,P'-bis[(1R,2R,3S,4R)-2,3,4-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L8 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

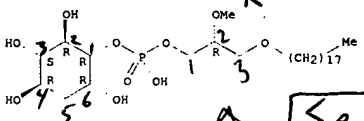
L8 ANSWER 15 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:1001605 CAPLUS
DOCUMENT NUMBER: 140:35923
TITLE: 3-Deoxy-D-myo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation thereof, and use for inhibition of cancer cell growth
INVENTOR(S): Kozikowski, Alan P.; Qiao, Lixin; Powis, Garth
PATENT ASSIGNEE(S): Arizona Board of Regents On Behalf of the University of Arizona, USA; Georgetown University School of Medicine
SOURCE: U.S., 24 pp., Cont.-in-part of U.S. Ser. No. 339,948.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6667340	B1	20031223	US 2001-879765	20010612
US 6245754	B1	20010612	US 1999-339948	19990625
EP 1574216	A1	20050914	EP 2005-76269	19990625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
US 2004192770	A1	20040930	US 2003-733115	20031211
PRIORITY APPLN. INFO.:			US 1998-90877P	P 19980626
			US 1999-339948	A2 19990625
			US 2000-223421P	P 20000807
			US 2000-223724P	P 20000808
			US 2000-235269P	P 20000926
			US 2000-235270P	P 20000926
			EP 1999-927339	A3 19990625
			US 2001-879765	A1 20010612

OTHER SOURCE(S): MARPAT 140:35923
AB The invention discloses the preparation and biol. activity of 3-deoxy-D-myo-inositol ether lipid analogs as inhibitors of phosphatidylinositol-3-kinase signaling and cancer cell growth. The compds. of the invention are useful as antitumor agents.
IT 253440-95-8P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation, and use for inhibition of cancer cell growth)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl

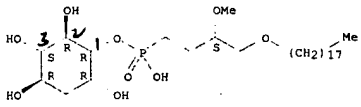
L8 ANSWER 15 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 253440-97-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyo-inositol ether lipid analogs as inhibitors of phosphatidyl myo-inositol cycle, preparation, and use for inhibition of cancer cell growth)
RN 253440-97-0 CAPLUS
CN Phosphonic acid, [(3S)-3-methoxy-4-(octadecyloxy)butyl]-, mono[(1R,2R,3S,4R,6R)-2,3,4,6-tetrahydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

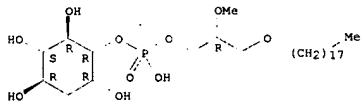


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 16 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:388780 CAPLUS
DOCUMENT NUMBER: 139:270468
TITLE: Specific inhibition of the Akt1 pleckstrin homology domain by D-3-deoxy-phosphatidyl-myo-inositol analogues
AUTHOR(S): Meuillet, Emmanuelle J.; Mahadevan, Daruka; Vankayalapati, Hariprasad; Berggren, Margareta; Williams, Ryan; Coon, Amy; Kozikowski, Alan P.; Powis, Garth
CORPORATE SOURCE: Arizona Cancer Center, University of Arizona, Tucson, AZ, 85724, USA
SOURCE: Molecular Cancer Therapeutics (2003), 2(4), 389-399
CODEN: MCTOCF; ISSN: 1535-7163
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Activation of Akt (protein kinase B), a Ser/Thr protein kinase that promotes cell survival, has been linked to tumorigenesis. Akt is activated by phosphorylation after binding of its pleckstrin homol. (PH) domain to plasma membrane phosphatidyl-myo-inositol-3-phosphates, formed by phosphoinositide-3-kinase. We report a novel strategy to inhibit Akt activation based on the use of D-3-deoxy-phosphatidyl-myo-inositols (DPIs) that cannot be phosphorylated on the 3-position of the myo-inositol ring. We have studied the DPIs, DPI 1-[(R)-2,3-bis(hexadecanoyloxy)propyl hydrogen phosphate], its ether lipid derivative DPI 1-[(R)-2-methoxy-3-octadecyloxypropyl hydrogen phosphate] (DPIEL), and its carbonate derivative DPI 1-[(R)-2-methoxy-3-octadecyloxypropyl carbonate]. We demonstrate in platelet-derived growth factor-stimulated mouse NIH3T3 cells that the DPIs bind to the PH domain of Akt, trapping it in the cytoplasm and thus preventing Akt activation. DPIEL did not inhibit myristylated-Akt, a constitutively active membrane-bound Akt expressed in NIH3T3 cells, and cell growth was not inhibited, unlike in wild-type NIH3T3 cells. Mol. modeling and docking studies show that DPIEL binds with much higher affinity to Akt's PH domain as compared with DPI and DPI 1-[(R)-2-methoxy-3-octadecyloxypropyl carbonate]. This study shows that the DPIs are a novel class of growth inhibitory agents with a novel mechanism of action through binding to the PH domain of Akt and inhibition of Akt activation.
IT 253440-95-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of Akt1 pleckstrin homol. domain by deoxyphosphatidyl-myo-inositol analogs)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 16 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



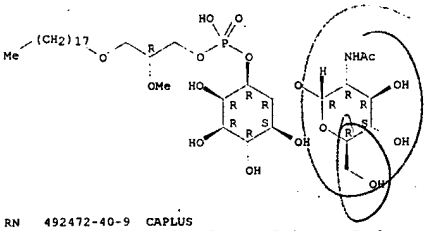
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 17 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:742972 CAPLUS
DOCUMENT NUMBER: 138:267573
TITLE: Specificities of Enzymes of Glycosylphosphatidylinositol Biosynthesis in Trypanosoma brucei and HeLa Cells
AUTHOR(S): Smith, Terry K.; Crossman, Arthur; Paterson, Michael J.; Borissow, Charles N.; Brimacombe, John S.; Ferguson, Michael A. J.
CORPORATE SOURCE: The School of Life Sciences, Division of Biological Chemistry & Molecular Microbiology, University of Dundee, Dundee, Scotland, DD1 5EH, UK
SOURCE: Journal of Biological Chemistry (2002), 277(40), 37147-37153
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of synthetic analogs of D-GlcNα1-6-D-myo-inositol-1-HPO4-sn-1,2-dipalmitoylglycerol, consisting of 22 variants of the d-GlcN or lipid components, were tested in trypanosomal and human (HeLa) cell-free systems. The assays measured the abilities of the analogs to act as substrates or inhibitors of the enzymes of glycosylphosphatidylinositol biosynthesis downstream of GlcNAc-phosphatidylinositol (GlcNAc-PI) de-N-acetylase. One compound, 4-deoxy-D-GlcNα1-6-D-myo-inositol-1-HPO4-sn-1,2-dipalmitoylglycerol, proved to be an inhibitor of both the trypanosomal and HeLa pathways, whereas 4-O-methyl-D-GlcNα1-6-D-myo-inositol-1-HPO4-sn-1,2-dipalmitoylglycerol and the 4'-epimer, D-GalN-α1-6-D-myo-inositol-1-HPO4-sn-1,2-dipalmitoylglycerol, were neither substrates nor inhibitors. The results with other analogs showed that the 6-OH of the α-D-GlcN residue is not required for substrate recognition in the trypanosomal and human pathways, whereas the 3-OH group is essential for both. Parasite-specific recognition of the β-linked analog D-GlcNβ1-6-D-myo-inositol-1-HPO4-sn-1,2-dipalmitoylglycerol is striking. This suggests that, like the GlcNAc-PI de-N-acetylase, the trypanosomal glycosylphosphatidylinositol α-mannosyltransferases, inositol acyltransferase and ethanolamine phosphate transferase, do not recognize the 2-, 3-, 4-, and 5-OH groups of the D-myo-inositol residue, whereas the human inositol acyltransferase and/or first α-mannosyltransferase recognizes one or more of these groups. All of the various lipid analogs tested served as substrates in both the trypanosomal and HeLa cell-free systems, suggesting that a precise lipid structure and stereochem. are not essential for substrate recognition. However, an analog containing a single C18:0 alkyl chain in place of sn-1,2-dipalmitoylglycerol proved to be a better substrate in the trypanosomal than in the HeLa cell-free system. These findings should have a bearing on the design of future generations of specific inhibitors of the trypanosomal glycosylphosphatidylinositol biosynthetic pathway.

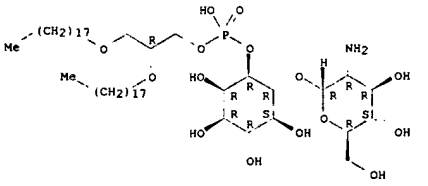
IT 363603-80-9 363603-81-0 363603-82-1
492472-40-9 492472-41-0
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(analogs of D-GlcNAc-PI permit anal. of substrate specificities for T. brucei and human glycosylphosphatidylinositol biosynthesis enzymes)

L8 ANSWER 17 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



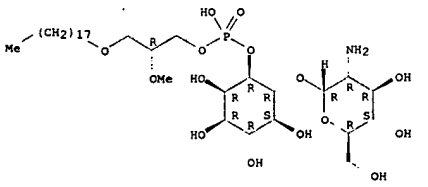
RN 492472-40-9 CAPLUS
CN D-myo-Inositol, 6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-, 1-[(2R)-2,3-bis(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



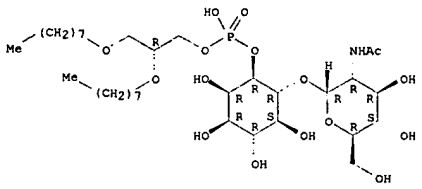
RN 492472-41-0 CAPLUS
CN D-myo-Inositol, 6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



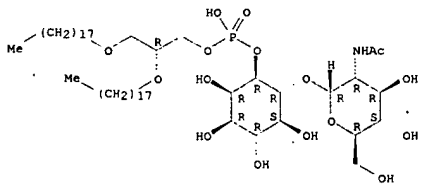
L8 ANSWER 17 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 363603-80-9 CAPLUS
CN D-myo-Inositol, 6-O-[2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-, 1-[(2R)-2,3-bis(octyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 363603-81-0 CAPLUS
CN D-myo-Inositol, 6-O-[2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-, 1-[(2R)-2,3-bis(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 363603-82-1 CAPLUS
CN D-myo-Inositol, 6-O-[2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

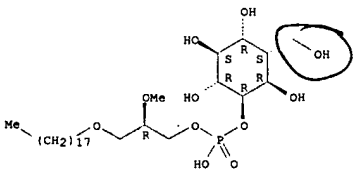
Absolute stereochemistry.

L8 ANSWER 17 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 18 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:255739 CAPLUS
DOCUMENT NUMBER: 137:140708
TITLE: Synthesis and biological activity of 3-hydroxy(phosphono)methyl-bearing phosphatidylinositol ether lipid analogues
AUTHOR(S): Sun, Haiying; Bapu Reddy, Gaddam; George, Clifford; Meuillet, Emmanuelle J.; Berggren, Margareta; Powis, Garth; Kozikowski, Alan P.
CORPORATE SOURCE: Department of Neurology, Drug Discovery Program, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Tetrahedron Letters (2002), 43(15), 2835-2838
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:140708
AB Two 3-hydroxy(phosphono)methyl-bearing phosphatidylinositol ether lipid analogs were synthesized and shown to be inhibitors of AKT and PI3-K. These compds. were also shown to inhibit the growth of HT-29 human colon cancer cells and MCF-7 human breast cancer cells.
IT 290812-35-0 290812-36-1
RL: PAC (Pharmacological activity); BIOL (Biological study)
(synthesis, AKT and PI3-K inhibition, and antitumor evaluation of 3-hydroxy(phosphono)methyl-bearing phosphatidylinositol ether lipid analogs)
RN 290812-35-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-1-(hydroxymethyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

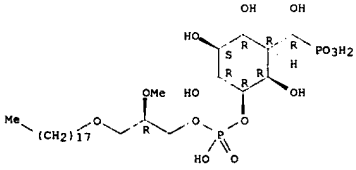
Absolute stereochemistry.



RN 290812-36-1 CAPLUS
CN D-myo-Inositol, 3-deoxy-3-(hydroxymethyl)-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

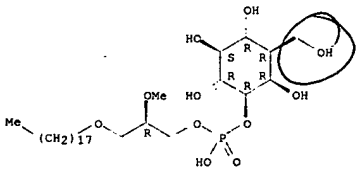
Absolute stereochemistry.

L8 ANSWER 18 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



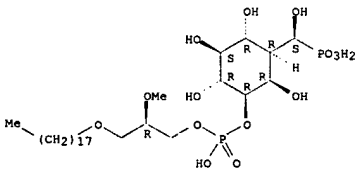
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 18 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 444902-97-0P 444902-98-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, AKT and PI3-K inhibition, and antitumor evaluation of 3-hydroxy(phosphono)methyl-bearing phosphatidylinositol ether lipid analogs)
RN 444902-97-0 CAPLUS
CN D-myo-Inositol, 3-deoxy-3-[(S)-hydroxyphosphonomethyl]-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



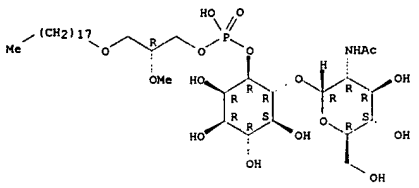
RN 444902-98-1 CAPLUS
CN D-myo-Inositol, 3-deoxy-3-[(R)-hydroxyphosphonomethyl]-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 19 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:544339 CAPLUS
DOCUMENT NUMBER: 135:269154
TITLE: Specificity of GlcNAc-PI de-N-acetylase of GPI biosynthesis and synthesis of parasite-specific suicide substrate inhibitors
AUTHOR(S): Smith, Terry K.; Crossman, Arthur; Borissow, Charles N.; Paterson, Michael J.; Dix, Alex; Brimacombe, John S.; Ferguson, Michael A. J.
CORPORATE SOURCE: Division of Biological Chemistry & Molecular Microbiology, The School of Life Sciences, University of Dundee, Dundee, DD1 5EH, UK
SOURCE: EMBO Journal (2001), 20(13), 3322-3332
CODEN: EMJODG; ISSN: 0261-4189
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The substrate specificities of Trypanosoma brucei and human (HeLa) GlcNAc-PI de-N-acetylases were determined using 24 substrate analogs. The results show the following. (i) The de-N-acetylases show little specificity for the lipid moiety of GlcNAc-PI. (ii) The 3'-OH group of the GlcNAc residue is essential for substrate recognition whereas the 6'-OH group is dispensable and the 4'-OH, while not required for recognition, cannot be epimerized or substituted. (iii) The parasite enzyme can act on analogs containing βGlcNAc or aromatic N-acyl groups, whereas the human enzyme cannot. (iv) Three GlcNR-PI analogs are de-N-acetylase inhibitors, one of which is a suicide inhibitor. (v) The suicide inhibitor most likely forms a carbamate or thiocarbamate ester to an active site hydroxy-amino acid or Cys or residue such that inhibition is reversed by certain nucleophiles. These and previous results were used to design two potent (IC50 = 8 nM) parasite-specific suicide substrate inhibitors. These are potential lead compds. for the development of anti-protozoan parasite drugs.
IT 363603-82-1
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(substrate specificities of T. brucei and human GlcNAc-PI de-N-acetylases promote design of parasite-specific suicide substrate inhibitors)
RN 363603-82-1 CAPLUS
CN D-myo-Inositol, 6-O-[2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

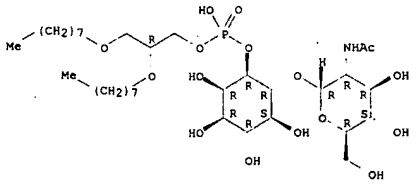
L8 ANSWER 19 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 363603-80-9 363603-81-0
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(substrate specificities of T. brucei and human GlcNAc-PI de-N-acetylases promote design of parasite-specific suicide substrate inhibitors)

RN 363603-80-9 CAPLUS
CN D-myo-Inositol, 6-O-[2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-, 1-[(2R)-2,3-bis(octyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

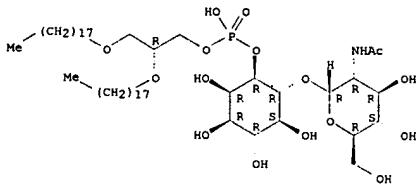
Absolute stereochemistry.



RN 363603-81-0 CAPLUS
CN D-myo-Inositol, 6-O-[2-(acetylamino)-2-deoxy-α-D-glucopyranosyl]-, 1-[(2R)-2,3-bis(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 19 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



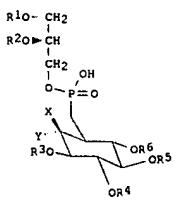
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 20 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:355095 CAPLUS
DOCUMENT NUMBER: 134:340656
TITLE: Preparation of glycerophosphatidylinositols as molecular probes and modulators for phosphatidylinositol-specific phospholipase C (PI-PLC) and phosphatidylinositol 3-kinase (PI 3-kinase)
INVENTOR(S): Aneja, Rajindra
PATENT ASSIGNEE(S): Nutrimed Biotech, USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6232486	B1	20010515	US 1997-872222	19970610
US 6384260	B1	20020507	US 2001-826396	20010403
PRIORITY APPLN. INFO.:			US 1996-19651P P	19960611
			US 1997-872222 A1	19970610

OTHER SOURCE(S): MARPAT 134:340656
GI



AB This invention provides analogs of phosphatidylinositol-phosphates I wherein at least one of R3, R4, R5, R6 is P(O)(OH)2, and wherein (a) X = F, Cl, Br, OC(O)R, OR, or OP(O)(OH)2, and Y = H; or X = Y = H; or (b) X = H, and Y = F, Cl, Br, OC(O)R, OR, or OP(O)(OH)2 ; or (c) X = Y = F or O; where R = alkyl, [especially Me or Et] alkenyl, alkynyl, ω-aminoalkyl, N-substituted-ω-aminoalkyl or N,N-disubstituted-ω-aminoalkyl; and wherein (d) R1 = RC(O) or R, R2 = R'C(O) or R' where R, R' = alkyl or alkenyl; and wherein (e) R3 = H, or P(O)(OH)2 (f) R4 = H, or P(O)(OH)2 (g) R5 = H, or P(O)(OH)2 (h) R6 = H, P(O)(OH)2, ω-aminoalkyl, ω-aminoalkenyt, ω.-sulthydrylalkyl, ω-carboxyalkyl, ω.-(4-azidosalicyl amido)-alkyl, alkyl-aminotluorophor,

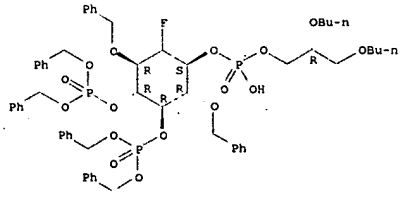
L8 ANSWER 20 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

alkyl-amidofluorophor, or alkyl-fluorophor, modified at one or more selected inositol-hydroxyls and optionally carrying reporter or anchoring groups attached in the lipid or the inositol residues, and, the synthetic intermediates and methods for the prepn. of these analogs. The analogs are useful as research reagents in biomedical studies related to structure, function and therapeuticals, including ref. materials for analyzing the metabolic products and efficacy studies of 2- and/or 3-hydroxyl modified inositols and phosphatidylinositols as drug candidates. Thus,
1D-2-deoxy-fluoro-1-O-(1',2'-di-O-palmitoyl-sn-glycero-3'-O-phospho)-myo/scyllo-inositol 4,5-bis-O-phosphate was prepd. as modulators for phosphatidylinositol-specific phospholipase C and phosphatidylinositol 3-kinase (no data).

IT 337955-75-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of glycerophosphatidylinositols as mol. probes and modulators for phosphatidylinositol-specific phospholipase C and phosphatidylinositol 3-kinase)

RN 337955-75-6 CAPLUS
CN D-myo-Inositol, 2-deoxy-2-fluoro-3,6-bis-O-(phenylmethyl)-, 4,5-bis[bis(phenylmethyl) phosphate] 1-[(2R)-2,3-dibutoxypropyl hydrogen phosphate], (2ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

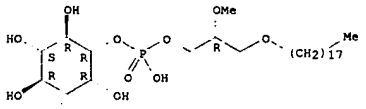
L8 ANSWER 21 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:242518 CAPLUS
DOCUMENT NUMBER: 135:101840
TITLE: High-performance liquid chromatographic analysis for a non-chromophore-containing phosphatidyl inositol analog, 1-[(1-O-octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol, using indirect UV detection
AUTHOR(S): He, J.; Cheung, A. P.; Wang, E.; Fang, K.; Liu, P.
CORPORATE SOURCE: SRI International, Menlo Park, CA, 94025-3493, USA
SOURCE: Journal of Chromatography, A (2001), 913(1-2), 355-363
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Phosphatidylinositide-3-kinase (PI3 kinase) is an important constituent of growth factor regulation. It is also involved in oncogene signaling pathways. An ether-containing phosphatidyl inositol(PI) analog, OMDPI, 1-[(1-O-octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol, is a potent inhibitor of this pathway and may be clin. useful in the treatment of a variety of neoplasms. OMDPI is currently being studied as an antitumor agent by the National Cancer Institute, NIH. OMDPI, a nonchromophore-containing PI analog, is not directly adaptable to the commonly used UV detection of HPLC. This paper reports the development and validation of an HPLC assay for OMDPI based on indirect UV detection, in which a UV-absorbing ion-pair reagent (the probe), protriptyline, is added to the mobile phase to induce a signal for the compound The method is sensitive (limit of detection <5 μL of 1 μg/mL or 5 ng), precise (relative standard deviation <2.5%), linear (r2 = 0.9995) and accurate (error<0.7%). It is superior to refractive index detection and evaporative light scattering detection in either sensitivity or linearity and does not require special equipment.

IT 253440-95-8, 1-[(1-O-Octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol
RL: ANT (Analyte); ANST (Analytical study)
(high-performance liquid chromatog. anal. for a non-chromophore-containing phosphatidyl inositol analog, 1-[(1-O-octadecyl-2-O-methyl-sn-glycero)-phospho]-1D-3-deoxy-myo-inositol, using indirect UV detection)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 21 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

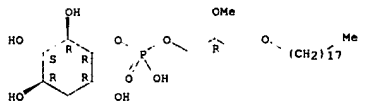
Inventors

L8 ANSWER 22 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:83663 CAPLUS
DOCUMENT NUMBER: 134:252547
TITLE: 3-Deoxy-3-substituted-D-myo-inositol imidazolyl ether lipid phosphates and carbonate as inhibitors of the phosphatidylinositol 3-kinase pathway and cancer cell growth
AUTHOR(S): Hu, Y.; Meuillet, E. J.; Berggren, M.; Powis, G.; Kozikowski, A. P.
CORPORATE SOURCE: Drug Discovery Program, Department of Neurology, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(2), 173-176
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:252547

AB 3-Modified D-myo-inositol imidazolyl ether lipid phosphates and a carbonate were synthesized and evaluated as inhibitors of PI3-K and Akt. These data are presented along with IC50 values for the inhibition of the growth of three cancer cell lines. 3-Modified D-myo-inositol imidazolyl ether lipid phosphates and a carbonate were synthesized and evaluated as inhibitors of PI3-K, Akt, and cancer cell growth.

IT 253440-95-8 290812-35-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of 3-deoxy-3-substituted-D-myo-inositol imidazolyl ether lipid phosphates and carbonate as inhibitors of the phosphatidylinositol 3-kinase pathway and cancer cell growth)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

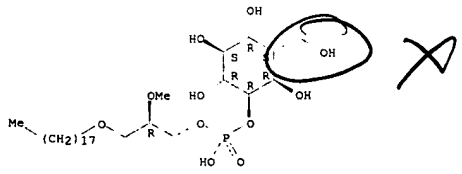


See 24

RN 290812-35-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-1-(hydroxymethyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 22 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

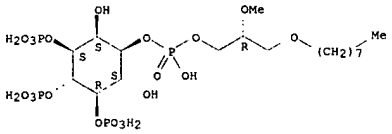
L8 ANSWER 23 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:893132 CAPLUS
DOCUMENT NUMBER: 134:308331
TITLE: A phosphatidylinositol 3,4,5-trisphosphate analogue with low serum protein-binding affinity
AUTHOR(S): Wang, D.-S.; Hsu, A.-L.; Chen, C.-S.
CORPORATE SOURCE: Division of Pharmaceutical Sciences, College of Pharmacy, University of Kentucky, Lexington, KY, 40536-0082, USA
SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(1), 133-139
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Phosphatidylinositol 3,4,5-trisphosphate (PIP3) plays an important role in the regulation of diverse physiol. functions. Recent evidence indicates that PIP3 is cell permeant, and can be added exogenously to modulate cellular responses. However, like many other phospholipids, PIP3 binds serum proteins with high affinity, resulting in rapid deactivation of this lipid second messenger. Our study indicates that bovine serum albumin (BSA) at concns. as low as 10 μg/mL abrogated the biol. activity of dipalmitoyl-PIP3. This nonspecific interaction with serum proteins hampers the use of PIP3 in biol. studies where serum is needed. We report here an ether-linked PIP3 analog, 1-O-(1-O-hexadecyl-2-O-methyl-sn-glycero-3-phosphoryl)-myo-inositol 3,4,5-trisphosphate (C16Me-PIP3), which displays low serum protein-binding affinity while retaining the biol. function of PIP3. The affinity of C16Me-PIP3 with BSA was two orders of magnitude lower than that of its dipalmitoyl-counterpart. Biochem. data indicate that C16Me-PIP3 was able to stimulate Ca2+ influx in T cells in the presence of moderate levels (up to 1 mg/mL) of BSA. Thus, C16Me-PIP3 may provide a useful tool to study the physiol. function of phosphoinositide (PI) 3-kinase in vivo.

IT 335163-59-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(a phosphatidylinositol 3,4,5-trisphosphate analog C16Me-PIP3 with low serum protein-binding affinity)
RN 335163-59-2 CAPLUS
CN D-myo-Inositol, 3,4,5-tris(dihydrogen phosphate) 1-[(2R)-3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 23 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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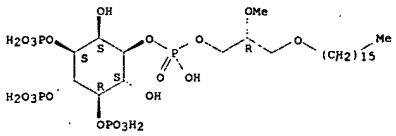
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

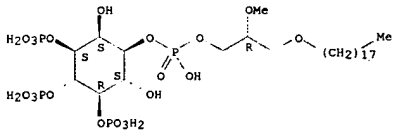
L8 ANSWER 23 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



X

IT 335163-60-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(a phosphatidylinositol 3,4,5-trisphosphate analog with low serum protein-binding affinity)
RN 335163-60-5 CAPLUS
CN D-myo-Inositol, 3,4,5-tris(dihydrogen phosphate) 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



X

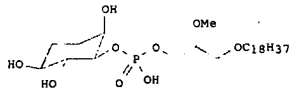
IT 335163-58-1P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(a phosphatidylinositol 3,4,5-trisphosphate analog with low serum protein-binding affinity)
RN 335163-58-1 CAPLUS
CN D-myo-Inositol, 3,4,5-tris(dihydrogen phosphate) 1-[(2R)-2-methoxy-3-(octyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Hu et al Inventors

L8 ANSWER 24 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:698487 CAPLUS
DOCUMENT NUMBER: 134:42338
TITLE: Synthesis and Akt kinase inhibitory properties of a 1d-3,4-dideoxyphosphatidylinositol ether lipid
AUTHOR(S): Hu, Y.; Meuillet, E. J.; Qiao, L.; Berggren, M. M.; Powis, G.; Kozikowski, A. P.
CORPORATE SOURCE: Department of Neurology, Drug Discovery Program, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Tetrahedron Letters (2000), 41(39), 7415-7418
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:42338
GI

IDS



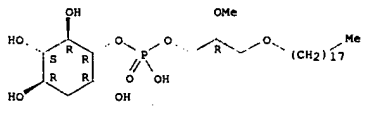
I

AB 1D-3,4-Dideoxyphosphatidylinositol ether lipid I (X = H) (DDPIEL), a PI analog, was synthesized through a sequence of protection/deprotection protocols and two Barton deoxygenation reactions, starting from L-(-)-quebrachitol. DDPIEL I is 18-fold more potent than its monodeoxy counterpart I (X = OH) (DPIEL) in the inhibition of PI3-K.

IT 253440-95-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and Akt kinase inhibitory properties of a 1d-3,4-dideoxyphosphatidylinositol ether lipid)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

R5 = H

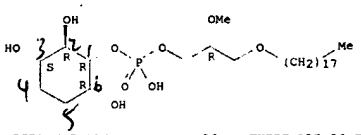


35

IT 310872-32-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and Akt kinase inhibitory properties of a

L8 ANSWER 24 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1d-3,4-dideoxyphosphatidylinositol ether lipid)
RN 310872-32-3 CAPLUS
CN Phosphoric acid, mono[(2R)-2-methoxy-3-(octadecyloxy)propyl] mono[(1R,2R,3S,5R,6R)-2,3,6-trihydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



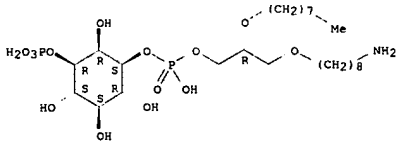
R4 R5 R6 = H

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

1,2,3,5-13,22,23
26, 34 135
37-40

R2 = OH
R3 = OH
R6 = OH

L8 ANSWER 25 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

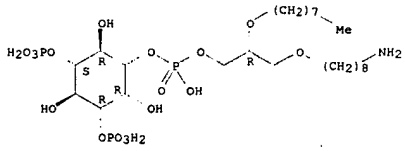


●2 Na

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 25 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:508645 CAPLUS
DOCUMENT NUMBER: 133:281991
TITLE: Preparation of L-α-phosphatidyl-D-myo-inositol 3-phosphate (3-PIP) and 3,5-bisphosphate (3,5-PIP2)
AUTHOR(S): Falck, J. R.; Krishna, U. M.; Capdevila, J. H.
CORPORATE SOURCE: Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX, 75390, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(15), 1711-1713
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:281991
AB Practical, asym. total syntheses of the title phospholipids from a readily
available myo-inositol derivative as well as short chain and cross-linked amino ether analogs are described.
IT 299216-97-0P 299216-99-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of L-α-phosphatidyl-D-myo-inositol 3-phosphate (3-PIP) and 3,5-bisphosphate (3,5-PIP2))
RN 299216-97-0 CAPLUS
CN D-myo-Inositol, 1-[(2R)-3-[(8-aminooctyl)oxy]-2-(octyloxy)propyl hydrogen phosphate] 3,5-bis(dihydrogen phosphate), tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●4 Na

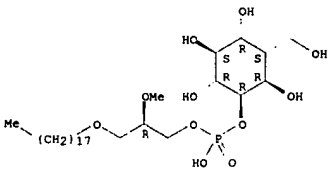
RN 299216-99-2 CAPLUS
CN D-myo-Inositol, 1-[(2R)-3-[(8-aminooctyl)oxy]-2-(octyloxy)propyl hydrogen phosphate] 3-(dihydrogen phosphate), disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 26 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:481805 CAPLUS
DOCUMENT NUMBER: 133:217271
TITLE: 3-(Hydroxymethyl)-Bearing Phosphatidylinositol Ether Lipid Analogues and Carbonate Surrogates Block PI3-K, Akt, and Cancer Cell Growth
AUTHOR(S): Hu, Youhong; Qiao, Lixin; Wang, Shaomeng; Rong, Suo-bao; Meuillet, Emmanuelle J.; Berggren, Margareta;
Gallegos, Alfred; Powis, Garth; Kozikowski, Alan P.
CORPORATE SOURCE: Drug Discovery Program Department of Neurology, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(16), 3045-3051
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phosphatidylinositol 3-kinase (PI3-K) phosphorylates the 3-position of phosphatidylinositol to give rise to three signaling phospholipids. Binding of the pleckstrin homol. (PH) domain of Akt to membrane PI(3)P's causes the translocation of Akt to the plasma membrane bringing it into contact with membrane-bound Akt kinase (PDK1 and 2), which phosphorylates and activates Akt. Akt inhibits apoptosis by phosphorylating Bad, thus promoting its binding to and blockade of the activity of the cell survival
factor Bcl-x. Herein we present the synthesis and biol. activity of several novel phosphatidylinositol analogs and demonstrate the ability of the carbonate group to function as a surrogate for the phosphate moiety. Due to a combination of their PI3-K and Akt inhibitory activities, the PI analogs proved to be good inhibitors of the growth of various cancer cell lines with IC50 values in the 1-10 μM range. The enhanced Akt inhibitory activity of the axial hydroxymethyl-bearing analog compared to its equatorial counterpart is rationalized based upon postulated differences in the H-bonding patterns of these compds. in complex with a homol. modeling generated structure of the PH domain of Akt. This work represents the first attempt to examine the effects of 3-modified PI analogs on these two crucial cell signaling proteins, PI3-K and Akt, in an
effort to better understand their cell growth inhibitory properties.
IT 290812-35-0P 290812-36-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure activity relations of phosphatidylinositol ether
lipid analogs and carbonate surrogates that block PI3-K, Akt kinase, and cancer cell growth)
RN 290812-35-0 CAPLUS
CN L-chiro-Inositol, 1-deoxy-1-(hydroxymethyl)-, 5-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

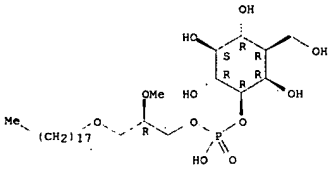
Absolute stereochemistry.

L8 ANSWER 26 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 290812-36-1 CAPLUS
CN D-myo-Inositol, 3-deoxy-3-(hydroxymethyl)-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 253440-95-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and structure activity relations of phosphatidylinositol ether lipid analogs and carbonate surrogates that block PI3-K, Akt kinase, and cancer cell growth)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

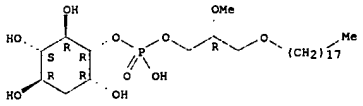
L8 ANSWER 27 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:15026 CAPLUS
DOCUMENT NUMBER: 132:59159
TITLE: Inhibitors of phosphatidyl-myo-insitol cycle for cancer treatment
INVENTOR(S): Kozikowski, Alan P.; Qioa, Lixin; Powis, Garth
PATENT ASSIGNEE(S): Georgetown University, USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000000206	A1	20000106	WO 1999-US12824	19990625
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9944271	A1	20000117	AU 1999-44271	19990607
CA 2335995	AA	20000106	CA 1999-2335995	19990625
EP 1119364	A1	20010801	EP 1999-927339	19990625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
EP 1574216	A1	20050914	EP 2005-76269	19990625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				

PRIORITY APPLN. INFO.: US 1998-90877P P 19980626
EP 1999-927339 A3 19990625
WO 1999-US12824 W 19990625

OTHER SOURCE(S): MARPAT 132:59159
AB The present invention relates to the preparation and biol. activity of 3-deoxy-D-myo-inositol ether lipid analogs as inhibitors of phosphatidylinositol-3-kinase signaling and cancer cell growth. The compds. of the present invention are useful as anti-tumor agents which effectively inhibit the growth of mammalian cells. For example, 1-O-octadecyl-2-O-methyl-sn-glycero-3-phospho-myo-inositol (OMDPI) administered by a 4 or 5 day daily i.p. schedule resulted in a 60% inhibition of the growth of human MCF-7 breast cancer and a 67% inhibition of the growth of HT-29 colon tumor xenografts implanted in SCID mice. The activity of OMDPI administered by a 10 day schedule provided 80% inhibition of the growth of MCF-7 xenografts.
IT 253440-95-8P 253440-97-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(inhibitors of phosphatidylinositol signaling for cancer treatment)

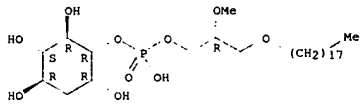
L8 ANSWER 26 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

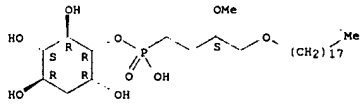
L8 ANSWER 27 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 253440-95-8 CAPLUS
CN D-myo-Inositol, 3-deoxy-, 1-[(2R)-2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 253440-97-0 CAPLUS
CN Phosphonic acid, [(3S)-3-methoxy-4-(octadecyloxy)butyl]-, mono[(1R,2R,3S,4R,6R)-2,3,4,6-tetrahydroxycyclohexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

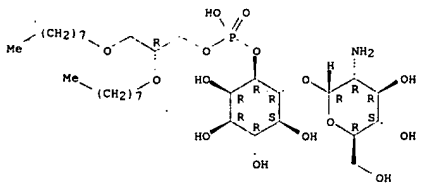


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 28 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:804893 CAPLUS
DOCUMENT NUMBER: 132:152056
TITLE: Parasite glycoconjugates. Part 10. Synthesis of some second-generation substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors
AUTHOR(S): Crossman, Arthur, Jr.; Brimacombe, John S.; Ferguson, Michael A. J.; Smith, Terry K.
CORPORATE SOURCE: Department of Chemistry, University of Dundee, Dundee, DD1 4HN, UK
SOURCE: Carbohydrate Research (1999), 321(1-2), 42-51
CODEN: CRBRAT; ISSN: 0008-6215
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1-D-6-O-(2-Amino-2-deoxy-α-D-glucopyranosyl)-2-O-octyl-myo-inositol 1-(1,2-di-O-hexadecanoyl-sn-glycerol 3-phosphate) (I) and the corresponding 2-O-hexadecyl-D-myo-inositol (II) have been prepared as substrate analogs of an early intermediate in the biosynthetic pathway of glycosylphosphatidylinositol (GPI) membrane anchors. 1-D-6-O-(2-Amino-2-deoxy-α-D-glucopyranosyl)-myo-inositol 1-(1,2-di-O-octyl-sn-glycerol 3-phosphate) has also been prepared as a substrate analog. Biol. evaluation of the analogs I and II revealed that they are neither substrates nor inhibitors of GPI biosynthetic enzymes in the human (HeLa) cell-free system but are potent inhibitors at different stages of GPI biosynthesis in the Trypanosoma brucei cell-free system.
IT 256922-40-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of some second-generation substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors)
RN 256922-40-4 CAPLUS
CN D-myo-Inositol, 6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-, 1-[(2R)-2,3-bis(octyloxy)propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L8 ANSWER 28 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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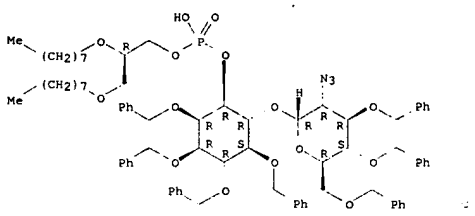
IT 256922-39-1P 257602-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of some second-generation substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors)
RN 256922-39-1 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis(octyloxy)propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 256922-38-0
CMF C80 H102 N3 O15 P

Absolute stereochemistry. Rotation (+).



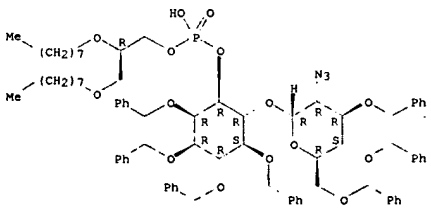
L8 ANSWER 28 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 121-44-8
CMF C6 H15 N

RN 257602-83-8 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis(octyloxy)propyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

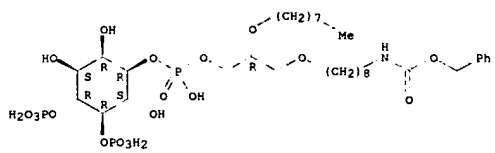


● Na

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 29 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:777603 CAPLUS
DOCUMENT NUMBER: 132:104405
TITLE: A synthesis of L-α-phosphatidyl-D-myo-inositol 4,5-bisphosphate (4,5-PIP2) and glyceryl lipid analogs
AUTHOR(S): Falck, J. R.; Krishna, U. Murali; Capdevila, Jorge H.
CORPORATE SOURCE: Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX, 75235, USA
SOURCE: Tetrahedron Letters (1999), 40(50), 8771-8774
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:104405
AB The title bioactive phosphatidylinositide and short-chain glyceryl lipid analogs were prepared from deoxyinosose 2, which was ultimately derived from 3-dehydroshikimic acid.
IT 255851-89-9P 255851-90-2P 255851-96-8P 255851-97-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of L-α-phosphatidyl-D-myo-inositol 4,5-bisphosphate (4,5-PIP2) and glyceryl lipid analogs)
RN 255851-89-9 CAPLUS
CN D-myo-Inositol, 4,5-bis(dihydrogen phosphate) 1-[(2R)-2-(octyloxy)-3-[[8-[[(phenylmethoxy)carbonyl]amino]octyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

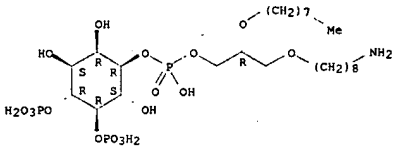
Absolute stereochemistry.



RN 255851-90-2 CAPLUS
CN D-myo-Inositol, 1-[(2R)-3-[(8-aminooctyl)oxy]-2-(octyloxy)propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

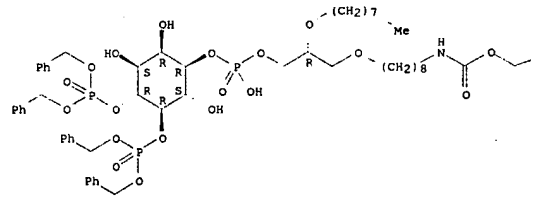
L8 ANSWER 29 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 255851-96-8 CAPLUS
CN D-myo-Inositol, 4,5-bis[bis(phenylmethyl) phosphate] 1-{(2R)-2-(octyloxy)-3-[{8-[[(phenylmethoxy)carbonyl]amino]octyl}oxy]propyl hydrogen phosphate} (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



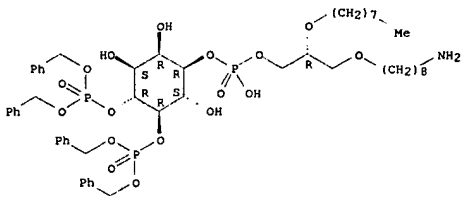
PAGE 1-B

Ph

RN 255851-97-9 CAPLUS
CN D-myo-Inositol, 1-{(2R)-3-[(8-aminooctyl)oxy]-2-(octyloxy)propyl hydrogen phosphate] 4,5-bis[bis(phenylmethyl) phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 29 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 30 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:584471 CAPLUS
DOCUMENT NUMBER: 131:335480
TITLE: A structural comparison of the total polar lipids from the human archaea Methanobrevibacter smithii and Methanosphaera stadtmanae and its relevance to the adjuvant activities of their liposomes
AUTHOR(S): Sprott, G. D.; Brisson, J.-R.; Dicaire, C. J.; Pelletier, A. K.; Deschatelets, L. A.; Krishnan, L.; Patel, G. B.
CORPORATE SOURCE: Institute for Biological Sciences, National Research Council of Canada, Ottawa, ON, Can.
SOURCE: Biochimica et Biophysica Acta, Molecular and Cell Biology of Lipids (1999), 1440(2-3), 275-288
CODEN: BBMLFG; ISSN: 1388-1981
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

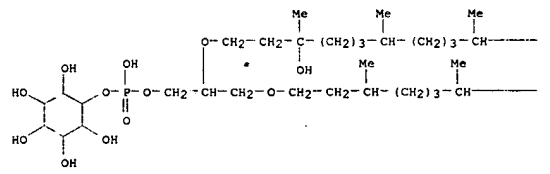
AB Mice were immunized with bovine serum albumin (BSA) entrapped within archaeosomes (i.e. liposomes) composed of the total polar lipids (TPL) from the two methanogenic archaea common to the human digestive tract. Methanobrevibacter smithii archaeosomes boosted serum anti-BSA antibody to titers comparable to those achieved with Freund's adjuvant, whereas Methanosphaera stadtmanae archaeosomes were relatively poor adjuvants. An explanation for this difference was sought by anal. of the polar lipid composition of each archaeobacterium. Fast atom bombardment mass spectrometry and NMR analyses of the purified lipids revealed a remarkable similarity in the ether lipid structures present in each TPL extract However, the relative amts. of each lipid species varied dramatically. The phospholipid fraction in M. stadtmanae TPL was dominated by archaetidylinositol (50 mol% of TPL) and the glycolipid fraction by β-Glcp-(1,6)-β-Glcp-(1,1)-archaeol (36 mol%), whereas in M. smithii exts., both caldarchaeol and archaeol lipids containing a phosphoserine head group were relatively abundant. Liposomes prepared from purified archaetidylinositol and from M. stadtmanae TPL supplemented with increasing amts. of phosphatidylserine elicited poor humoral responses to encapsulated BSA. A dramatic loss in the adjuvanticity of M. smithii archaeosomes was seen upon incorporation of 36 mol% of the uncharged lipid diglucosyl archaeol and, to a lesser extent, of 50 mol% of archaetidylinositol. Interestingly, the relative rates of uptake of M. smithii and M. stadtmanae archaeosomes by phagocytic cultures in vitro were similar. Thus, the lipid composition may influence archaeosome adjuvanticity, particularly a high diglucosyl archaeol and/or archaetidyl inositol content, resulting in a low adjuvant activity.

IT 134067-43-9 249756-42-1
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(structure-immunostimulation study of polar lipid archaeosomes of Methanobrevibacter smithii and Methanosphaera stadtmanae)

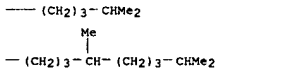
RN 134067-43-9 CAPLUS
CN D-myo-Inositol, 1-[(2S)-2-[[(7R,11R)-3-hydroxy-3,7,11,15-tetramethylhexadecyl]oxy]-3-[[(3R,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L8 ANSWER 30 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



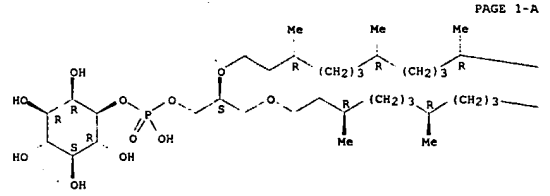
PAGE 1-B



RN 249756-42-1 CAPLUS
CN D-myo-Inositol, 1-[(2S)-2,3-bis[[(3R,7R,11R,15R)-3,7,11,15-tetramethylhexadecyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

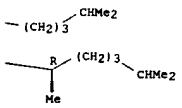
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 30 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

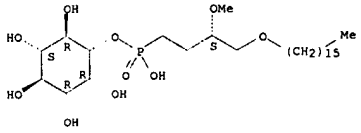
PAGE 1-B

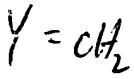


REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 31 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
methoxybutyl]phosphonate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.





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REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

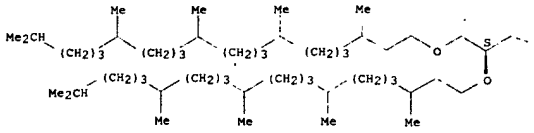
L8 ANSWER 31 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:256247 CAPLUS
DOCUMENT NUMBER: 131:53696
TITLE: Effects of a water-soluble antitumor ether phosphonoinositide, D-myo-inositol 4-(hexadecyloxy)-3(S)-methoxybutanephosphonate (C4-PI), on inositol lipid metabolism in breast epithelial cancer cell lines
AUTHOR(S): Lin, Weiyang; Leung, Lawrence W.; Bae, Yun Soo; Bittman, Robert; Arthur, Gilbert
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, University of Manitoba, Winnipeg, MB, R3E 0W3, Can.
SOURCE: Biochemical Pharmacology (1999), 57(10), 1153-1158
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have demonstrated previously that D-myo-inositol 4-(hexadecyloxy)-3(S)-methoxybutanephosphonate (C4-PI), an isosteric phosphonate analog of phosphatidylinositol developed to inhibit inositol lipid metabolism, was unable to inhibit phosphatidylinositol (PI) 3-kinase activity. We now report the effects of the compound on other aspects of inositol metabolism We demonstrated that C4-PI inhibits the activity of purified recombinant PI-phospholipase C-β (PLC-β) at all concns. tested; it enhanced the activity of PI-PLC-γ and PI-PLC-δ at low concns. (10 μM), while severely inhibiting their activities at higher concns. In the breast cancer cell lines MCF-7 (estrogen receptor pos.) and MDA-MB-468 (estrogen receptor neg.), C4-PI had no effect on the uptake of D-myo-inositol but severely inhibited its incorporation into PI. In spite of the drastic decrease in PI synthesis, C4-PI did not affect the levels of inositol incorporated into phosphatidylinositol 4,5-bisphosphate (PIP2) in the cells. In vitro assays showed that C4-PI inhibited PI synthase activity (inhibition of 35% at 50 μM) but had little effect on PI 4-kinase activity (inhibition of 13% at 150 μM). C4-PI inhibited the proliferation of MCF-7 and MDA-MB-468 cell lines with IC50 values of 12 and 18 μM. Taken together, the results suggest that the accumulation of [3H]inositol in PIP2 in cells incubated with C4-PI may be due to the inhibition of PIP2 hydrolysis in the cells with no effect on its synthesis. The role of these C4-PI-induced effects in the mechanism of growth inhibition by C4-PI remains to be established.
IT 211696-22-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of a water-soluble antitumor ether phosphonoinositide C4-PI on inositol lipid metabolism in breast epithelial cancer cells)
RN 211696-22-9 CAPLUS
CN D-myo-Inositol, 1-[hydrogen [(3S)-4-(hexadecyloxy)-3-

L8 ANSWER 32 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:89860 CAPLUS
DOCUMENT NUMBER: 130:249205
TITLE: A novel phosphoglycolipid archaetidyl(glucosyl)inositol with two sesterterpanyl chains from the aerobic hyperthermophilic archaeon Aeropyrum pernix K1
AUTHOR(S): Morii, Hiroyuki; Yagi, Hiromasa; Akutsu, Hideo; Nomura, Norimichi; Sako, Yoshihiko; Koga, Yosuke
CORPORATE SOURCE: Department of Environmental Management, University of Occupational and Environmental Health, Kitakyushu, 807-8555, Japan
SOURCE: Biochimica et Biophysica Acta, Molecular and Cell Biology of Lipids (1999), 1436(3), 426-436
CODEN: BBMLFG; ISSN: 1388-1981
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structures of two novel polar lipids (AGI and AI) of an aerobic hyperthermophilic archaeon, Aeropyrum pernix, were elucidated. AGI and AI were the only two major lipids and accounted for 91 mol% and 9 mol%, resp., of total polar lipids of this organism. The core lipid of A. pernix total lipids consisted solely of 2,3-di-O-sesterterpanyl-sn-glycerol (C25,25-archaeol). The mol. wts. of the free acid forms of AGI and AI were shown by FAB-mass spectrometry to be 1196 and 1034, resp. AI was completely hydrolyzed by phosphatidylinositol-specific phospholipase C, while AGI was not hydrolyzed at all under the same condition for the hydrolysis of AI. The molar ratio of phosphate, myo-inositol, and glucose in AGI was 1.0:0.97:0.95. The positions of linkages between myo-inositol and glucose, and between myo-inositol and phosphate in AGI were determined by NMR analyses of intact AGI and glucosylinositol prepared from AGI. Finally, it was concluded that the structures of AGI and AI were 2,3-di-O-sesterterpanyl-sn-glycerol-1-phospho-1'-(2'-O-α-D-glucosyl)-myo-inositol (C25,25-archaetidyl(glucosyl)inositol) and 2,3-di-O-sesterterpanyl-sn-glycerol-1-phospho-myo-inositol (C25,25-archaetidylinositol), resp. This is the first example that a core lipid of whole polar lipids is composed of only one species C25,25-archaeol in one organism and that glucosylinositol is found in a polar lipid as a polar head group.
IT 221461-67-2P 221461-68-3P
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(structure determination of two novel polar lipids from the aerobic hyperthermophilic archaeon Aeropyrum pernix)
RN 221461-67-2 CAPLUS
CN myo-Inositol, 2-O-α-D-glucopyranosyl-, 1-[(2S)-2,3-bis[(3,7,11,15,19-pentamethyleicosyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

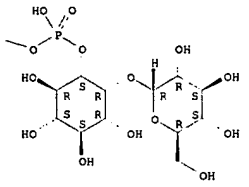
Absolute stereochemistry.

L8 ANSWER 32 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



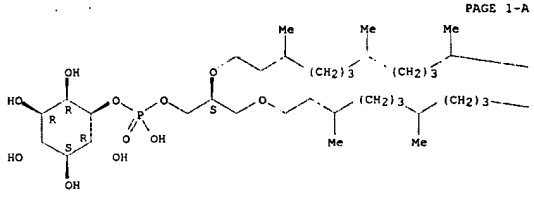
PAGE 1-B



RN 221461-68-3 CAPLUS
CN myo-Inositol, 1-[(2S)-2,3-bis[(3,7,11,15,19-pentamethyleicosyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

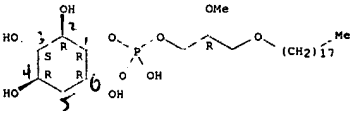
PAGE 1-A



IDS

L8 ANSWER 33 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:503329 CAPLUS
DOCUMENT NUMBER: 129:254488
TITLE: 3-Deoxy-D-myo-inositol 1-phosphate, 1-phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol-3-kinase signaling and cancer cell growth
AUTHOR(S): Qiao, Lixin; Nan, Fajun; Kunkel, Mark; Gallegos, Alfred; Powis, Garth; Kozikowski, Alan P.
CORPORATE SOURCE: Drug Discovery Program, Georgetown University Medical Center, Washington, DC, 20007, USA
SOURCE: Journal of Medicinal Chemistry (1998), 41(18), 3303-3306
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and the bioactivity of several ratically designed phosphatidylinositol analogs are presented. The studies have been directed toward the synthesis of 3-substituted myo-inositol derivs. to selectively block the effects of myo-inositol-derived second messengers on cell proliferation and transformation while living other aspects of myo-inositol signalling uneffected. This strategy may offer a basis for the selective control of cancer growth without disrupting the function of normal cells.
IT 213388-41-1P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyoinositol phosphate, phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol kinase signaling and cancer cell growth)
RN 213388-41-1 CAPLUS
CN chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3R)-3-methoxy-4-(octadecyloxy)butyl]phosphate] (9CI) (CA INDEX NAME)

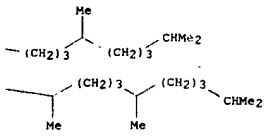
Relative stereochemistry.



IT 213388-42-2P 213408-29-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(deoxymyoinositol phosphate, phosphonate, and ether lipid analogs as inhibitors of phosphatidylinositol kinase signaling and cancer cell growth)
RN 213388-42-2 CAPLUS
CN chiro-Inositol, 1-deoxy-, 5-[hydrogen [(3S)-3-methoxy-4-

L8 ANSWER 32 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

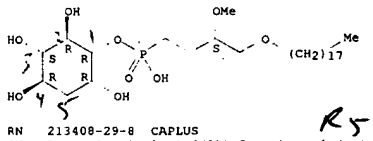
PAGE 1-B



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 33 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(octadecyloxy)butyl]phosphonate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

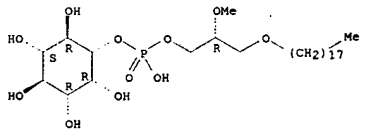


Y = CH2

RN 213408-29-8 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2-methoxy-1-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

R5 = H

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

1,2,3,5-13,23,24,27,28,37-40

X=O
Y=CH2

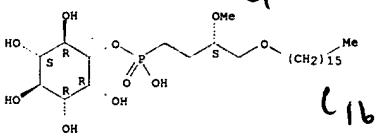
L8 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:400088 CAPLUS
DOCUMENT NUMBER: 129:185938
TITLE: A novel water-soluble phosphonate analog of phosphatidylinositol, D-myo-inositol 4-(hexadecyloxy)-3(S)-methoxybutanephosphonate (C4-PI), inhibits epithelial cell proliferation and is a substrate but not an inhibitor of phosphatidylinositol 3-kinase
AUTHOR(S): Leung, Lawrence W.; Lin, Weiyang; Richard, Christina; Bittman, Robert; Arthur, Gilbert
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Queens College of The City University of New York, Flushing, NY, 11367, USA
SOURCE: Journal of Liposome Research (1998), 8(2), 213-224
CODEN: JLREE7; ISSN: 0898-2104
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB D-Myo-Inositol 4-(hexadecyloxy)-3(S)-methoxybutanephosphonate (C4-PI), a water soluble isosteric phosphonate analog of phosphatidylinositol (PI) that is not a substrate of phosphatidylinositol-specific phospholipase C isoenzymes, was synthesized and was found to be phosphorylated by phosphatidyl-inositol 3-kinase (PI 3-kinase) activity immunopptd. from insulin-stimulated cells. The extent of phosphorylation of C4-PI was similar to or greater than that of phosphatidylinositol, especially at higher concns. Since C4-PI is very water soluble, it is an attractive tool for assaying PI kinases in vitro as no detergent or sonication is required in contrast to assays with the long-chain PI which forms micelles. C4-PI was, at best, a poor inhibitor of PI 3-kinase activity (IC50 > 150 μM). C4-PI exhibited antiproliferative properties against the neuroblastoma cell lines SK-N-SH and SK-N-MC and the kidney carcinoma A498 cell line (IC50 20-40 μM) but had minimal effect on the proliferation of the drug-resistant ovarian adenocarcinoma OVCAR-3 line. These results indicate that the antiproliferative effect of C4-PI is unlikely to arise via inhibition of the PI 3-kinase signaling pathways in cells. However, the possibility that phosphorylated C4-PI products interfere in PI 3-kinase cell signaling pathways cannot be ruled out.

IT 211696-22-9P
RL: ARG (Analytical reagent use); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of a novel water-soluble phosphonate analog of phosphatidylinositol (C4-PI) that inhibits epithelial cell proliferation and is a substrate but not an inhibitor of phosphatidylinositol 3-kinase)
RN 211696-22-9 CAPLUS
CN D-myo-Inositol, 1-[hydrogen [(3S)-4-(hexadecyloxy)-3-methoxybutyl]phosphonate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



C16

Y=CH2

● Na

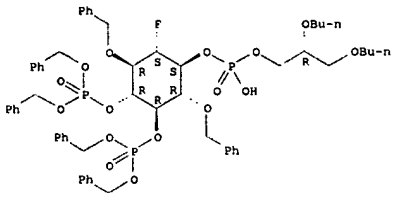
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 35 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:330471 CAPLUS
DOCUMENT NUMBER: 129:67941
TITLE: Synthesis of 2-deoxy-2-fluoro-phosphatidylinositol-4,5-bisphosphate and analogs: probes and modulators of the mammalian PI-PLCS
AUTHOR(S): Aneja, Sarla G.; Ivanova, Pavlina T.; Aneja, Rajindra
CORPORATE SOURCE: Functional Lipids Division, Langmuir Laboratory, Nutrimed Biotech, Cornell University Research Park, Ithaca, NY, 14850, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(9), 1061-1064
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An approach to synthesis of 2-modified phosphatidylinositol-4,5-bisphosphates, which are substrate analogs useful as probes and modulators of the PI-PLC enzyme family, is described and illustrated for the dibutyl-2-deoxy-2-fluoro analog, a probe designed for delineating substrate and PI-PLC interactions by X-ray crystallog.

IT 208844-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deoxyfluorophosphatidylinositol bisphosphate and analogs as probes and modulators of the mammalian PI-PLCS)
RN 208844-99-9 CAPLUS
CN D-scyllo-Inositol, 1-deoxy-1-fluoro-3,6-bis-O-(phenylmethyl)-, 4,5-bis[bis(phenylmethyl) phosphate] 2-[(2R)-2,3-dibutoxypropyl hydrogen phosphate] (9CI) (CA INDEX NAME)

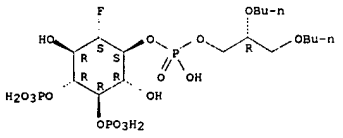
Absolute stereochemistry.



IT 208845-00-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deoxyfluorophosphatidylinositol bisphosphate and analogs as probes and modulators of the mammalian PI-PLCS)
RN 208845-00-5 CAPLUS

L8 ANSWER 35 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN D-scyllo-Inositol, 1-deoxy-1-fluoro-, 2-[(2R)-2,3-dibutoxypropyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

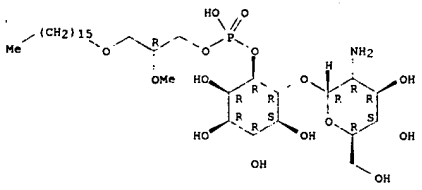
L8 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:663354 CAPLUS
DOCUMENT NUMBER: 127:307581
TITLE: Parasite glycoconjugates. Part 7. Synthesis of further substrate analogs of early intermediates in the biosynthetic pathway of glycosylphosphatidylinositol membrane anchors
AUTHOR(S): Crossman, Arthur, Jr.; Brimacombe, John S.; Ferguson, Michael A. J.
CORPORATE SOURCE: Department of Chemistry, University of Dundee, Dundee, DD1 4HN, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (18), 2769-2774
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Substrate analogs of 1D-6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-myo-inositol 1-[sn-2,3-bis(myristoyloxy)propyl phosphate], an early intermediate in the bio-preparation of glycosylphosphatidylinositol (GPI) membrane anchors, have been prepared for biol. evaluation with the α-(1→4)-D-mannosyltransferase of the protozoan parasite Trypanosoma brucei. The analog α-D-GlcpNH2-(1→6)-2-OMe-PI is a substrate for the protozoan α-(1→4)-D-mannosyltransferase but not for the corresponding mammalian enzyme, whereas the analogs, in which the fatty-acid groups of the natural substrate are replaced by alkyl groups, are acceptable substrates for both the protozoan and mammalian enzymes.

IT 197369-71-4P 197369-72-5P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation of glycosylphosphatidylinositol membrane anchors as substrates for the protozoan mannosyltransferase)

RN 197369-71-4 CAPLUS
CN D-myo-Inositol, 6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-, 1-[(2R)-3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

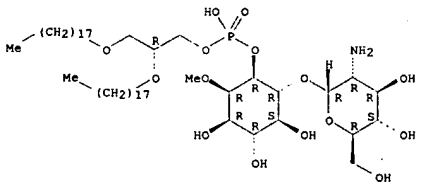


● Na

L8 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 197369-72-5 CAPLUS
CN D-myo-Inositol, 6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-2-O-methyl-, 1-[(2R)-2,3-bis(octadecyloxy)propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● Na

IT 197369-86-1P 197369-88-3P 197385-16-3P 197385-17-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of glycosylphosphatidylinositol membrane anchors as substrates for the protozoan mannosyltransferase)

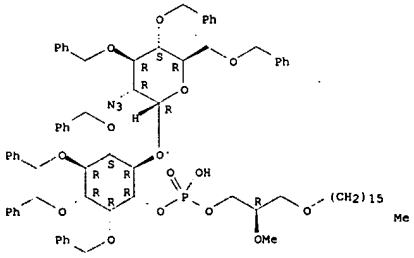
RN 197369-86-1 CAPLUS

L8 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 197369-85-0
CMF C81 H104 N3 O15 P

Absolute stereochemistry. Rotation (+).



CM 2

CRN 121-44-8
CMF C6 H15 N

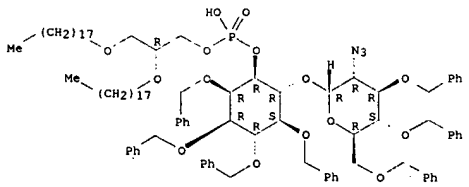
RN 197369-88-3 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-bis(octadecyloxy)propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 197369-87-2
CMF C100 H142 N3 O15 P

Absolute stereochemistry. Rotation (+).

L8 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



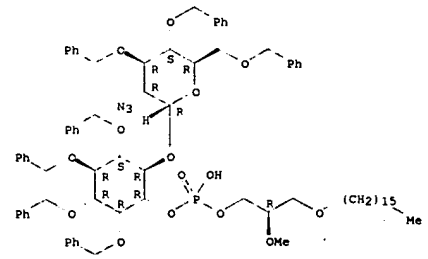
CM 2

CRN 121-44-8
CMF C6 H15 N

RN 197385-16-3 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



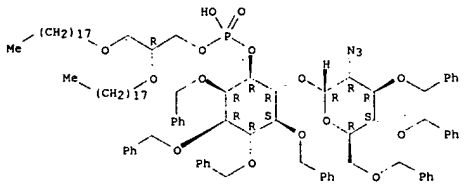
L8 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

● Na

RN 197385-17-4 CAPLUS
CN D-myo-Inositol, 6-O-[2-azido-2-deoxy-3,4,6-tris-O-(phenylmethyl)-α-D-glucopyranosyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, 1-[(2R)-2,3-(octadecyloxy)propyl hydrogen phosphate], sodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

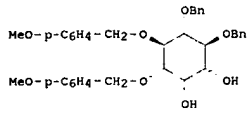


● Na

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 37 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:589694 CAPLUS
DOCUMENT NUMBER: 127:234517
TITLE: Intracellular second messengers: synthesis of L-α-phosphatidyl-D-myo-inositol 3,4-bisphosphate and analogs
AUTHOR(S): Reddy, K. Kishta; Ye, Jianhua; Falck, J. R.; Capdevila, Jorge H.
CORPORATE SOURCE: Departments of Biochemistry and Pharmacology, University of Texas Southwestern Medical Center, Dallas, TX, 75235-9038, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(16), 2115-2116
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

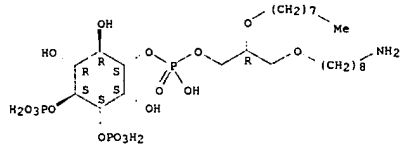


I

AB Concise syntheses of the title phospholipid as well as a water soluble, short
chain diester and a cross-linkable aminodiether analog utilized chiral inositol I.
IT 195303-15-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of L-α-phosphatidyl-D-myo-inositol bisphosphate and analogs)
RN 195303-15-2 CAPLUS
CN D-myo-Inositol, 1-[(2R)-3-[(8-aminooctyl)oxy]-2-(octyloxy)propyl hydrogen phosphate] 3,4-bis(dihydrogen phosphate), pentasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 37 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



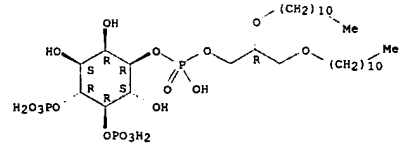
●5 Na

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:188994 CAPLUS
DOCUMENT NUMBER: 126:277683
TITLE: Synthesis of a tritium-labeled diether analog of phosphatidylinositol 4,5-bisphosphate
AUTHOR(S): Chen, Jian; Prestwich, Glenn D.
CORPORATE SOURCE: Department of Chemistry, University at Stony Brook, Stony Brook, NY, 11794-3400, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1997), 39(3), 251-258
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of 1-(1,2,O-diundecyl-sn-glycerylphosphoryl) 4,5-D-myo-inosityl bisphosphate and its tritiated analog are described. The convergent synthesis employed optically-pure inositol and glycerol derivs. In the final step, hydrogenation of an alkenyl chain gave the saturated diether PIP2 and tritiation gave the high-specific activity, tritium-labeled analog.
IT 188950-61-0P 188950-62-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of a tritium-labeled diether analog of phosphatidylinositol bisphosphate)
RN 188950-61-0 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis(undecyloxy)propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate), pentasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

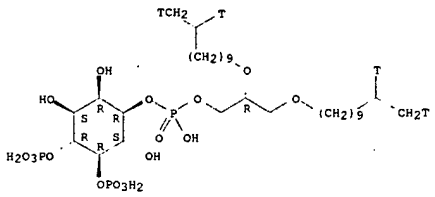


●5 Na

RN 188950-62-1 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis(undecyl-10,11-t2-oxy)propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate), pentasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



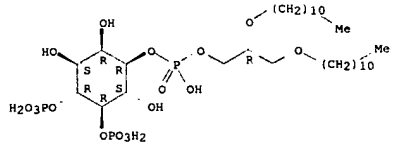
●5 Na

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 39 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:187721 CAPLUS
DOCUMENT NUMBER: 126:275448
TITLE: Regulation of AP-3 function by inositides. Identification of phosphatidylinositol 3,4,5-trisphosphate as a potent ligand
AUTHOR(S): Hao, Weihua; Tan, Zheng; Prasad, Kondury; Reddy, K. Kishta; Chen, Jian; Prestwich, Glenn D.; Falck, John R.; Shears, Stephen B.; Lafer, Eileen M.
CORPORATE SOURCE: Department Molecular Medicine, University Texas Health
Science Center San Antonio, San Antonio, TX, 78245, USA
SOURCE: Journal of Biological Chemistry (1997), 272(10), 6393-6398
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB As part of the growing effort to understand the role inositol phosphates and inositol lipids play in the regulation of vesicle traffic within nerve
terminals, we determined whether or not the synapse-specific clathrin assembly
protein AP-3 can interact with inositol lipids. We found that soluble dioctanoyl-phosphatidylinnositol 3,4,5-trisphosphate (DiC8PtdIns(3,4,5)P3)
was only 7.5-fold weaker a ligand than D-myo-inositol hexakisphosphate in assays that measured the displacement of D-myo-[3H]inositol hexakisphosphate. In functional assays we found that both of these ligands inhibited clathrin assembly, but DiC8-PtdIns(3,4,5)P3 was more potent and exhibited a larger maximal effect. We also examined the structural features of DiC8-PtdIns(3,4,5)P3 that establish specificity. Dioctanoyl-phosphatidylinositol 3,4-bisphosphate, which does not have a 5-phosphate, and 4,5-O-bisphosphoryl-D-myo-inosityl 1-O-(1,2-O-diundecyl)-
sn-3-glycerylphosphate, which does not have a 3-phosphate, were, resp., 2-fold and 4-fold less potent than DiC8-PtdIns(3,4,5)P3 as inhibitors of clathrin assembly. Deacylation of DiC8-PtdIns(3,4,5)P3 reduced its affinity for AP-3 almost 20-fold, and also dramatically lowered its ability to inhibit clathrin assembly. The deacylated products of the soluble
derivs. of phosphatidylinositol 3,4-bisphosphate and phosphatidylinositol 4,5-bisphosphate were both not significant inhibitors of clathrin assembly. It therefore appears that the interactions of inositides with AP-3 should not be considered simply in terms of electrostatic effects of the highly charged phosphate groups. Ligand specificity appears also to be mediated by hydrophobic interactions with the fatty-acyl chains of the inositol lipids.
IT 188885-39-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); BIOL (Biological study)
(phosphatidylinositol 3,4,5-trisphosphate as a potent ligand in regulation of AP-3 function by inositides)

L8 ANSWER 39 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 188885-39-4 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis(undecyloxy)propyl hydrogen phosphate] 4,5-bis(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

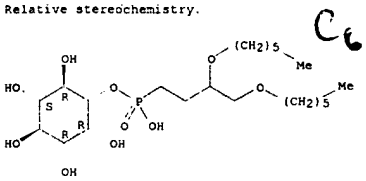


Ryan et al

L8 ANSWER 40 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:618920 CAPLUS
DOCUMENT NUMBER: 126:16188
TITLE: Synthesis, structure-activity relationships, and the effect of polyethylene glycol on inhibitors of phosphatidylinositol-specific phospholipase C from Bacillus cereus
AUTHOR(S): Ryan, Margret; Smith, Miles P.; Vinod, Thottumkara K.;
Lau, Wai Leung; Keana, John F. W.; Griffith, O. Hayes
CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene,
OR, 97403-1229, USA
SOURCE: Journal of Medicinal Chemistry (1996), 39(22), 4366-4376
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Substrate analog inhibitors of B. cereus phosphatidylinositol-specific phospholipase C (PI-PLC) were synthesized and screened for their suitability to map the active site region of the enzyme by protein crystallog. Analogs of the natural substrate, phosphatidylinositol (PI), were designed to examine the importance of the lipid portion and the inositol phosphate head group for binding to the enzyme. The synthetic compds. contained pentyl, hexyl, or hexanoyl and octyl lipid chains at the
sn-1 and sn-2 positions of the glycerol backbone and phosphonoinositol, phosphonic acid, Me phosphonate, phosphatidic acid, or Me phosphate at the
sn-3 position. The most hydrophobic compound, dioctyl Me phosphate, was also the best inhibitor with an IC50 of 12 μM. In a series of dihexyl lipids, compds. with phosphonoinositol head groups inhibited more strongly
than those that did not contain inositol but were otherwise identical. A short-chain lipid with a phosphonoinositol head group was found to be a competitive inhibitor and the most potent in this series with an IC50 of 18 μM (Ki =14 μM). Analogs with dihexyl chains were better inhibitors than those with dihexanoyl chains, presumably because the ether-linked lipids were more hydrophobic than the ester-linked lipids. No appreciable difference in inhibition was found between a phosphonoinositol lipid and the corresponding difluorophosphonoinositol lipid. Inositols and inositol derivs. that did not contain lipid moieties
showed IC50 values .apprx.3 orders of magnitude above those of the short-chain lipids. In this group, glucosaminyl(α1→6)-D-myo-inositol inhibited more strongly than did myo-inositol, which in turn was a better inhibitor than inositol phosphate. The addition of polyethylene glycol (PEG-600) resulted in a marked decrease in inhibition by the short-chain lipids, but had little effect on the water-soluble head group analogs. This was accounted for in terms of solubilization of the amphipathic inhibitors by PEG. Since PEG is required in crystallization, these
data indicate that the best strategy for obtaining enzyme inhibitor complexes is to start by cocrystg. PI-PLC with the head group analogs. The next step is to synthetically add the shortest possible hydrophobic moieties to the analogs and cocrystallize these with the enzyme. This strategy may be applicable to other lipolytic enzymes.
IT 184180-05-0 184180-06-1
RL: BAC (Biological activity or effector, except adverse); BSU

L8 ANSWER 40 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
study, unclassified); BIOL (Biological study)
(structure-activity relations of inhibitors of phosphatidylinositol-specific phospholipase C from Bacillus cereus)
RN 184180-05-0 CAPLUS
CN myo-Inositol, 1-[hydrogen [3,4-bis(hexyloxy)butyl]phosphonate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

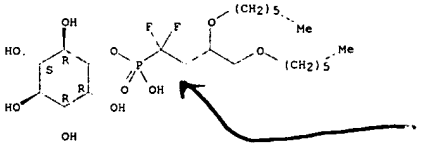


C6

Y = CH2

RN 184180-06-1 CAPLUS
CN myo-Inositol, 1-[hydrogen [1,1-difluoro-3,4-bis(hexyloxy)butyl]phosphonate] (9CI) (CA INDEX NAME)

Relative stereochemistry.



C6

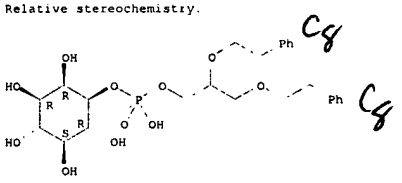
Y = CF2

REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 41 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:565322 CAPLUS
DOCUMENT NUMBER: 125:268946
TITLE: Inhibition of phosphatidylinositol-specific phospholipase C: Studies on synthetic substrates, inhibitors and a synthetic enzyme
AUTHOR(S): Vizitiu, Dragos; Kriste, Angela G.; Campbell, A. Stewart; Thatcher, Gregory R. J.
CORPORATE SOURCE: Dep. Chemistry, Queen's Univ., Kingston, ON, K7L 3N6, Can.
SOURCE: Journal of Molecular Recognition (1996), 9(2), 197-209
CODEN: JMORE4; ISSN: 0952-3499
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:268946
AB Enzyme inhibition studies on phosphatidylinositol-specific phospholipase C
(PI-PLC) from Bacillus cereus were performed in order to gain an understanding of the mechanism of the PI-PLC family of enzymes and to aid inhibitor design. Inhibition studies on two synthetic cyclic phosphonate analogs (1,2) of inositol cyclic-1:2-monophosphate (cIP), glycerol-2-phosphate, and vanadate were performed using natural phosphatidylinositol (PI) substrate in Triton X100 co-micelles and an NMR assay. Further inhibition studies on PI-PLC from B. Cereus were performed
using a chromogenic, synthetic PI analog (DPG-PI), an HPLC assay, and Aerosol-OT (AOT), phytic acid, and vanadate as inhibitors. For purposes of comparison, a model PI-PLC enzyme system was developed employing a synthetic Cu(II)-metallomicelle and a further synthetic PI analog (IPP-PI). The studies employing natural PI substrate in Triton X100 co-micelles and synthetic DPG-PI in the absence of surfactant indicate three classes of PI-PLC inhibitors: (1) active-site directed inhibitors (e.g. 1,2); (2) water-soluble polyanions (e.g. tetravanadate, phytic acid);
(3) surfactant anions (e.g. AOT). Three modes of mol. recognition are indicated to be important: (1) active site mol. recognition; (2) recognition at an anion-recognition site, which may be the active site, and (3) interfacial (or hydrophobic) recognition which may be exploited to
increase affinity for the anion-recognition site in anionic surfactants such as AOT. The most potent inhibition of PI-PLC was observed by tetravanadate and AOT. The metallomicelle model system was observed to mimic
PI-PLC in reproducing transesterification of the PI analog substrate to yield cIP as product and in showing inhibition by phytic acid and AOT.
IT 182144-14-5P 182144-18-9P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC
(Process)
(as synthetic substrate; inhibition of Bacillus cereus phosphatidylinositol-specific phospholipase C using synthetic and non-synthetic substrates, inhibitors, and synthetic enzyme)
RN 182144-14-5 CAPLUS

L8 ANSWER 41 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN myo-Inositol, 1-[2,3-bis(2-phenylethoxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

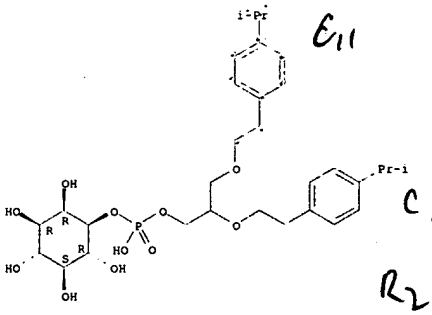
Relative stereochemistry.



C8 C8

RN 182144-18-9 CAPLUS
CN myo-Inositol, 1-[2,3-bis[2-[4-(1-methylethyl)phenyl]ethoxy]propyl hydrogen
phosphate] (9CI) (CA INDEX NAME)

Relative stereochemistry.



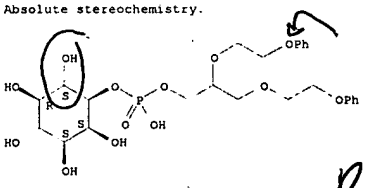
C11

R2=OH

1-3, SAME, SAME

L8 ANSWER 42 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:281812 CAPLUS
DOCUMENT NUMBER: 125:58907
TITLE: A metallomicelle enzyme model for phospholipase C catalysis and inhibition
AUTHOR(S): Kriste, Angela G.; Vizitiu, Dragos; Thatcher, Gregory R. J.
CORPORATE SOURCE: Dep. Chemistry, Queen's Univ., Kingston, ON, K7L 3N6, Can.
SOURCE: Chemical Communications (Cambridge) (1996), (8), 913-914
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A CuII metallo-micelle mimics phospholipase C enzymes in catalysis and inhibition of transesterification of inositol phosphate diesters.
IT 178157-13-6
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(copper(II) metallo-micelle enzyme model for phospholipase C catalysis and inhibition)
RN 178157-13-6 CAPLUS
CN D-myo-Inositol, 3-[2,3-bis(2-phenoxyethoxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

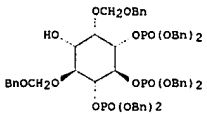


X

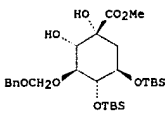
R7 R1

R2 = (S)-OH = O-Ak-OH

L8 ANSWER 43 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:579010 CAPLUS
DOCUMENT NUMBER: 123:9807
TITLE: Intracellular Mediators: Synthesis of L-α-Phosphatidyl-D-myo-inositol 3,4,5-Trisphosphate and Glyceryl Ether Analogs
AUTHOR(S): Reddy, K. Kishta; Saady, Mourad; Falck, J. R.; Whited, Gregg
CORPORATE SOURCE: Southwestern Medical Center, University of Texas, Dallas, TX, 75235, USA
SOURCE: Journal of Organic Chemistry (1995), 60(11), 3385-90
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:9807
GI



I

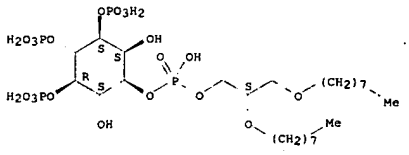


II

AB 1-α-Phosphatidyl-D-myo-inositol 3,4,5-trisphosphate (3,4,5-PIP3), the most prominent member of a new class of intracellular second messengers, and two ether analogs were conveniently prepared from the differentially functionalized D-myo-inositol intermediate I which was ultimately derived from the unique cyclitol precursor dehydroshikimic acid. Critical transformations included the stereoselective hydride reduction of the shikimate ketone, exclusive osmylation from the α-face to give II, controlled enolization and dioxirane epoxidn. with in situ rearrangement affording the corresponding ketone. Dioctanoyl 3,4,5-PIP3 and its dioctyl ether analog 9b selectively activated the δ, ε, and η-isotypes of PKC.
IT 163563-78-8P 163563-79-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of phosphatidyldinositol trisphosphate and glyceryl ether analogs)
RN 163563-78-8 CAPLUS
CN D-myo-Inositol, 1-[(2S)-2,3-bis(octyloxy)propyl hydrogen phosphate] 3,4,5-tris(dihydrogen phosphate), heptasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

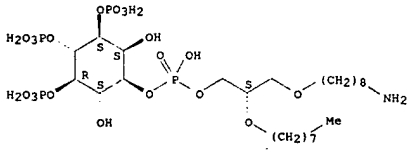
L8 ANSWER 43 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



●7 Na

RN 163563-79-9 CAPLUS
CN D-myo-Inositol, 1-[(2S)-3-[(8-aminooctyl)oxy]-2-(octyloxy)propyl hydrogen phosphate] 3,4,5-tris(dihydrogen phosphate), heptasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●7 Na

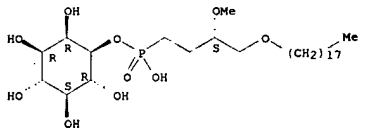
L8 ANSWER 44 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:278613 CAPLUS
DOCUMENT NUMBER: 122:123155
TITLE: Phosphonates as for treatment of cancer or inflammation or other diseases
INVENTOR(S): Salari, Hassan; Bittman, Robert
PATENT ASSIGNEE(S): University of British Columbia, Can.
SOURCE: U.S., 14 pp. Cont.-in-part of U.S. 5,219,845.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5369097	A	19941129	US 1993-59170	19930504
US 5219845	A	19930615	US 1992-835732	19920211
US 5506217	A	19960409	US 1994-337958	19941110
PRIORITY APPLN. INFO.:			US 1991-692452 B2	19910425
			US 1992-835732 A2	19920211
			US 1993-59170 A2	19930504

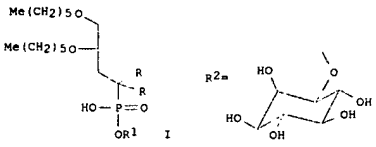
OTHER SOURCE(S): MARPAT 122:123155
AB The invention pertains to the synthesis and use as therapeutic agents of a group of substances with a glycerol backbone or aliphatic chain structure linked to a phosphorus atom and a polar head group. Depending on the polar head group, the substance has anti-cancer, anti-inflammatory, anti-allergy or anti-cardiovascular disease properties. Compds. of the formula C(OR1)C(OR2)C(CH2)nOP(O)(O-)R3 and C(OR1)C(OR2)C(CH2)nP(O)(O-)R3 [n = 0-14; and R1 = C12-20 alkyl; R2 = Me; R3 = inositol analog head group, (CH2)m N+(CH3)3 (m = 2-10), serine head group, ethanolamine head group], or of the formula C(OR1)C(OR2)C(CH2)nP(O)(O-)OR3 [R1, R2 as above; n = 0, 1; R3 = (CH2)mN+(CH3)3 (m = 2-10)] are disclosed. Also disclosed are the synthesis and use as therapeutic agents of a group of substances that have no glycerol backbone but have an aliphatic chain structure linked directly to a phosphorus atom of the general formula RP(O)(O-)OR' (R = long-chain alkyl, e.g. hexadecyl or octadecyl; R' = head group, e.g. choline, glycerol, inositol, ethanolamine, or serine). Anti-tumor, anti-inflammatory, cardiovascular, etc. activities of compds. of the invention are presented.
IT 160850-39-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(phosphonates as for treatment of cancer or inflammation or other diseases)
RN 160850-39-5 CAPLUS
CN myo-Inositol, 1-[hydrogen [3-methoxy-4-(octadecyloxy)butyl]phosphonate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

L8 ANSWER 44 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L8 ANSWER 45 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:115140 CAPLUS
DOCUMENT NUMBER: 122:240236
TITLE: Synthesis of isosteric and isopolar phosphonate substrate analogs designed as inhibitors for phosphatidylinositol-specific phospholipase C from Bacillus cereus
AUTHOR(S): Vinod, Thottumkara K.; Griffith, O. Hayes; Keana, John F. W.
CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403, USA
SOURCE: Tetrahedron Letters (1994), 35(39), 7193-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

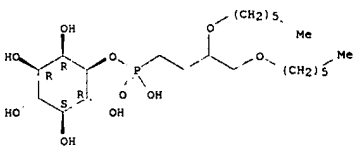


AB The synthesis of the isosteric phosphonate substrate analog inhibitor I (R = H, R1 = R2) and the isopolar difluoromethylenephosphonate inhibitor I (R = F, R1 = R2) for phosphatidylinositol-specific phospholipase C (PI-PLC) from Bacillus cereus is described. The key step involved a trichloroacetonitrile mediated condensation between the inositol derivative and the corresponding phosphonic acids I (R = H, F, R1 = H) to establish the central P-O bond in these inhibitors.
IT 162315-19-7P 162315-20-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phosphatidylinositols via trichloroacetonitrile mediated condensation of inositol with phosphonic acid)
RN 162315-19-7 CAPLUS
CN D-myo-Inositol, 2,3-cyclohexylidene-4,5,6-tris-O-(methoxymethyl)-, hydrogen [3,4-bis(hexyloxy)butyl]phosphonate, ammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

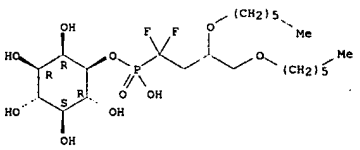
L8 ANSWER 45 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(CA INDEX NAME)

Absolute stereochemistry.

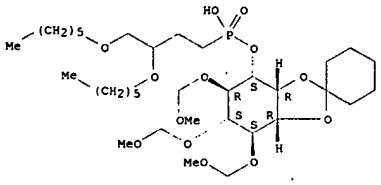


RN 162315-09-5 CAPLUS
CN D-myo-Inositol, 1-[hydrogen [1,1-difluoro-3,4-bis(hexyloxy)butyl]phosphonate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



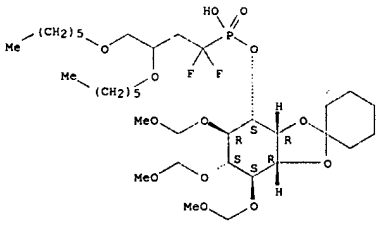
L8 ANSWER 45 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● NH_3

RN 162315-20-0 CAPLUS
CN D-myo-Inositol, 2,3-cyclohexylidene-4,5,6-tris-O-(methoxymethyl)-, hydrogen [1,1-difluoro-3,4-bis(hexyloxy)butyl]phosphonate, ammonium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

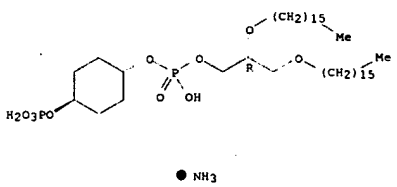


● NH_3

IT 162315-08-4P 162315-09-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phosphatidylinositols via trichloroacetonitrile mediated condensation of inositol with phosphonic acid)
RN 162315-08-4 CAPLUS
CN D-myo-Inositol, 1-[hydrogen [3,4-bis(hexyloxy)butyl]phosphonate] (9CI)

L8 ANSWER 46 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:100000 CAPLUS
DOCUMENT NUMBER: 122:127265
TITLE: Inhibition of human erythrocyte membrane phosphatidylinositol 4-kinase by phospholipid analogs
AUTHOR(S): Young, R. C.; Downes, C. P.; Jones, M.; Milliner, K. J.; Rana, K. K.; Ward, J. G.
CORPORATE SOURCE: SmithKline Beecham Pharmaceuticals, Welwyn/Hertfordshire, AL6 9AR, UK
SOURCE: European Journal of Medicinal Chemistry (1994), 29(7-8), 537-49
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Analogs of phosphatidylinositol (PtdIns, 1) have been synthesized to investigate the structural requirements for inhibition of a PtdIns 4-kinase obtained from human erythrocyte membranes. While the presence of either D-1 or D-3 stereochem. in the inositol moiety greatly influences the degree of inhibition produced by PtdIns analogs, the stereochem. of the glycerol moiety is of little consequence. Neither structural feature, however, makes a significant contribution to binding affinity. Competitive inhibitory activity was retained (or even enhanced) in substantially simpler analogs consisting of 1 or 2 hydrocarbon chains attached to a charged phosphate head group, such as in the phosphatidic acids. The observation that the phosphatidylinositol 4-phosphate (PtdIns 4P) and phosphatidic acid analogs inhibit PtdIns 4-kinase may suggest that such species have a regulatory role in PtdIns turnover.
IT 161105-07-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of phospholipid analogs and evaluation as phosphatidylinositol 4-kinase inhibitors)
RN 161105-07-3 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] mono[4-(phosphonooxy)cyclohexyl] ester, monoammonium salt, [1(R)-trans]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

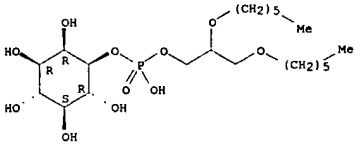


● NH_3

IT 161003-15-2P 161003-16-3P 161003-19-6P

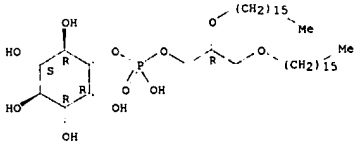
L8 ANSWER 46 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
161105-04-0P 161105-08-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of phospholipid analogs and evaluation as phosphatidylinositol 4-kinase inhibitors)
RN 161003-15-2 CAPLUS
CN myo-Inositol, 1-[2,3-bis(hexyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 161003-16-3 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis(hexadecyloxy)propyl hydrogen phosphate], (R)- (9CI) (CA INDEX NAME)

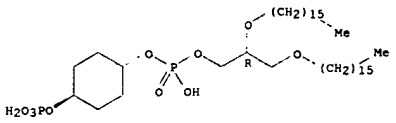
Absolute stereochemistry.



RN 161003-19-6 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] mono[4-(phosphonooxy)cyclohexyl] ester, [1(R)-trans]- (9CI) (CA INDEX NAME)

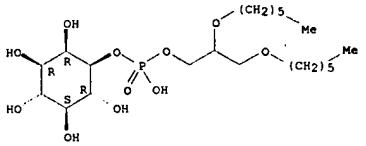
Absolute stereochemistry.

L8 ANSWER 46 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 161105-04-0 CAPLUS
CN myo-Inositol, 1-[2,3-bis(hexyloxy)propyl hydrogen phosphate], monoammonium
salt (9CI) (CA INDEX NAME)

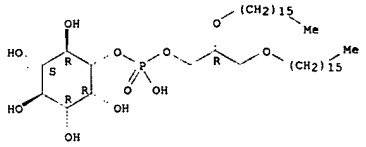
Relative stereochemistry.



● NH_3

RN 161105-08-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis(hexadecyloxy)propyl hydrogen phosphate], monoammonium salt, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

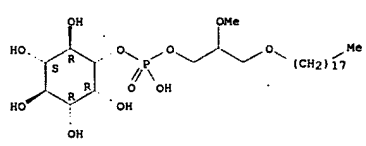


● NH_3

L8 ANSWER 46 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L8 ANSWER 47 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:671278 CAPLUS
DOCUMENT NUMBER: 121:271278
TITLE: Selective effect of O-alkyl lysophospholipids on the growth of a human lung giant cell carcinoma cell line
AUTHOR(S): Goto, Isao; Hozumi, Motoo; Honma, Yoshio
CORPORATE SOURCE: Res. Inst., Saitama Cancer Cent., Ina, 362, Japan
SOURCE: Anticancer Research (1994), 14(2A), 357-62
CODEN: ANTRD4; ISSN: 0250-7005
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Various alkyl ether lipids were synthesized and their effects on the proliferation of human lung carcinoma cells were examined The proliferation of Lu-65, a giant cell carcinoma cell line, was significantly decreased with 1 μg/mL (3-tetradecyloxy-2-methoxy) propyl-2-trimethylammonioethyl phosphate, while the proliferation of Lu-99, another giant cell carcinoma cell line, was unaffected even by treatment with 5 μg/mL of the alkyl lysophospocholine. Adenocarcinoma PC-9 and small cell carcinoma H-69 cells were also fairly resistant to the alkyl ether lipid. Among the alkyl ether lipids tested, 3-nonadecyloxy-2-methoxypropyl 2-trimethylammonioethyl phosphate was the most effective in inhibiting the growth of Lu-65 cells. However, the pyridinioethyl derivative had higher selectivity for the growth of Lu-65 cells than the choline derivative The sensitivity of Lu-65 cells to the alkyl lysophospholipids was similar to that of human myeloid leukemia cells including HL-60. However, the sensitivity of Lu-65 cells to the other types of alkyl ether lipids were much lower than those of HL-60 cells. These results indicate that Lu-65 cells are selectively sensitive to alkyl lysophospholipids.
IT 112924-43-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(structure effect on antiproliferation activity of alkyl lysophospholipids in human lung giant cell carcinoma cells)
RN 112924-43-3 CAPLUS
CN myo-Inositol, 1-(2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Relative stereochemistry.

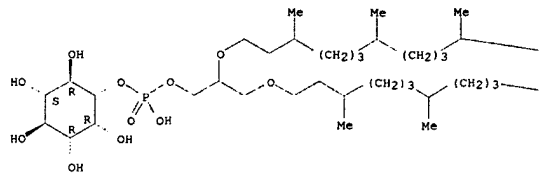


L8 ANSWER 48 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:318972 CAPLUS
DOCUMENT NUMBER: 120:318972
TITLE: Asymmetrical topology of diether- and tetraether-type polar lipids in membranes of Methanobacterium thermoautotrophicum cells
AUTHOR(S): Morii, Hiroyuki; Koga, Yosuke
CORPORATE SOURCE: Dep. Chem., Univ. Occup. and Environ. Health, Kitakyushu, 807, Japan
SOURCE: Journal of Biological Chemistry (1994), 269(14), 10492-7
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The distribution of diether polar lipids between the inner and outer leaflets of the membrane of Methanobacterium thermoautotrophicum was investigated by comparing the orientation of tetraether polar lipids, which constitute a monolayer in the same membrane. Three kinds of reactions were employed for intact cells or protoplasts and unsealed membrane fragments prepared from the organism: glycosidase digestion for glycolipids, NaIO4 oxidation for glycolipids and inositol lipids, and trinitrophenylation for aminophospholipids. The results indicated that (a) most gentiobiose residues of both diether and tetraether polar lipids were mainly oriented to the cytoplasmic surface of the membrane; and (c) approx. 80% of arachaetidylethanolamine (diether type) was distributed in the outer leaflet of the membrane bilayer, while only 25% of the ethanolamine residue of gentiobiosyl caldarchaetidylethanolamine (tetraether type) was oriented to the outer surface of the membrane. These results, except for ethanolamine lipids, are consistent with the hypothesis that the tetraether polar lipids are synthesized from the corresponding diether polar lipid precursors that have been already substituted by polar groups in the membrane by head-to-head condensation without rearrangement of lipids.
IT 111955-11-4, Archaetidylinositol
RL: PROC (Process)
(of Methanobacterium thermoautotrophicum cell membrane, topol. distribution of)
RN 111955-11-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

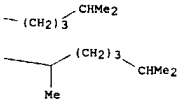
Absolute stereochemistry.

L8 ANSWER 48 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



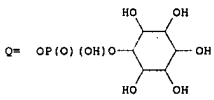
PAGE 1-B



L8 ANSWER 49 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:37805 CAPLUS
DOCUMENT NUMBER: 120:37805
TITLE: Skin cosmetics containing 1,2-diphytanylglycerols and polyalcohols
INVENTOR(S): Sumida, Yasushi; Tokunaga, Kazunobu
PATENT ASSIGNEE(S): Kanebo Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05170639	A2	19930709	JP 1991-356955	19911224
PRIORITY APPLN. INFO.:			JP 1991-356955	19911224

GI

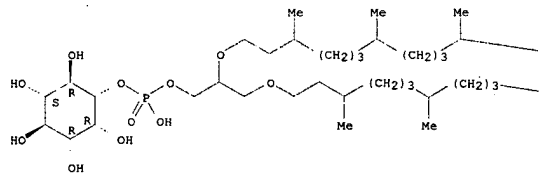


AB Skin cosmetics contain Me2CH(CH2)2[CH2CHMe(CH2)2]3OCH2CH[O[(CH2)2CHMeCH2]3(CH2)2CHMe2]CH2X [I; X = OP(O)(O-)O(CH2)2N+Me3, OP(O)(O-)O(CH2)2NH3+, OP(O)(O-)CH2CH(CO2H)NH3+, Q, OP(O)(OH)2 or its salts] and water-soluble polyalcs. The cosmetics show moisturizing effect and are not sticky. A skin lotion containing 0.9 weight% 1,2-diphytanylglycero-3-phosphoethanolamine was formulated.
IT 150447-38-4
RL: BIOL (Biological study)
(moisturizing cosmetics containing polyalcs. and)
RN 150447-38-4 CAPLUS
CN myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

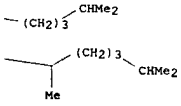
Relative stereochemistry.

L8 ANSWER 49 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



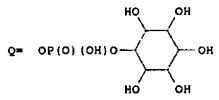
PAGE 1-B



L8 ANSWER 50 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:588297 CAPLUS
DOCUMENT NUMBER: 119:188297
TITLE: Topical preparations containing 1,2-diphytanylglycerols
INVENTOR(S): Sumida, Yasushi; Tokunaga, Kazunobu
PATENT ASSIGNEE(S): Kanebo Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05170640	A2	19930709	JP 1991-356956	19911224
PRIORITY APPLN. INFO.:			JP 1991-356956	19911224

GI

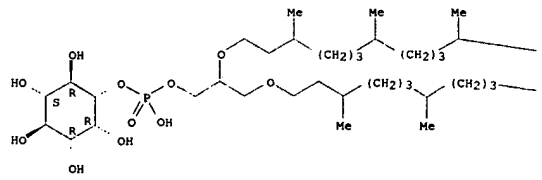


AB Topical prepns. contain Me2CH(CH2)2[CH2CHMe(CH2)2]3OCH2CH[O[(CH2)2CHMeCH2]3(CH2)2CHMe2]CH2X [X = OP(O)(O-)O(CH2)2N+Me3, OP(O)(O-)O(CH2)2NH3+, OP(O)(O-)CH2CH(CO2H)NH3+, Q, OP(O)(OH)2 or its salts] and active ingredients, e.g. blood circulation improvers, cell-activating agents, skin-lightening agents. A topical preparation containing 0.1 weight% vitamin E nicotinate (I) and 10.0 weight% 1,2-diphytanylglycero-3-phosphocholine was applied to the skin of rabbits to show 60% increase in the blood flow rate 2 h later, vs. 10%, for a control preparation containing I itself.
IT 150447-38-4
RL: BIOL (Biological study)
(topical prepns. containing active ingredients and, as enhancer)
RN 150447-38-4 CAPLUS
CN myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

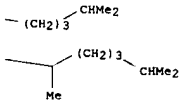
Relative stereochemistry.

L8 ANSWER 50 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



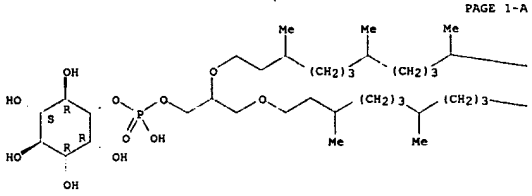
PAGE 1-B



L8 ANSWER 51 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:555735 CAPLUS
DOCUMENT NUMBER: 119:155735
TITLE: Tetraether type polar lipids increase after logarithmic growth phase of Methanobacterium thermoautotrophicum in compensation for the decrease of diether lipids
AUTHOR(S): Morii, Hiroyuki; Koga, Yosuke
CORPORATE SOURCE: Dep. Chem., Univ. Occup. Environ. Health, Kitakyushu, 807, Japan
SOURCE: FEMS Microbiology Letters (1993), 109(2-3), 283-7
CODEN: FMLED7; ISSN: 0378-1097
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The ratios of tetraether to diether type lipids in the total lipid during cell growth in batch cultures of M. thermoautotrophicum ΔH (DSM 1053) were examined The proportion of tetraether type lipids to the total lipid was .apprx.80% during the log phase, and at the onset of the transient phase it began to rise up to .apprx.93%. It was kept almost constant at that level throughout the stationary phase. The polar lipid composition changed with the age of the cell culture. The proportions of all the diether type polar lipids were lower and the levels of all tetraether type polar lipids were higher in the stationary phase than in the log phase. On the other hand, the composition of polar head groups, irresp. of the core lipids, was nearly constant in both growth phases measured so far despite the change in core lipid composition
IT 111955-11-4, Archaetidylinositol
RL: BIOL (Biological study)
(of Methanobacterium thermoautotrophicum in logarithmic growth phase)
RN 111955-11-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

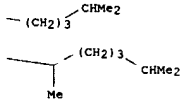
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 51 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



L8 ANSWER 52 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:22543 CAPLUS
DOCUMENT NUMBER: 118:22543
TITLE: Preparation of intermediates for glycosylphosphatidylinositol anchors
INVENTOR(S): Ogawa, Tomoya; Muragata, Tsutomu; Saito, Hiromitsu
PATENT ASSIGNEE(S): Institute of Physical and Chemical Research, Japan; Kyowa Hakko Kogyo Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04120089	A2	19920421	JP 1990-240960	19900911
PRIORITY APPLN. INFO.:			JP 1990-240960	19900911

GI

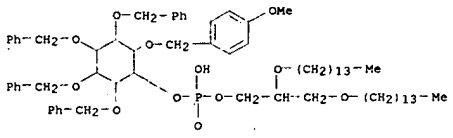
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title intermediates, e.g. I and II, are prepared E.g., I was prepared in
4 steps from the protected hexopyranose diacetate III via reaction with p-MeOC6H4OH in methylene chloride containing CF3SO3SiMe3, hydrolysis, reaction
with benzyl alc., ClP[N(CHMe2)2]2, and HOCH2CH2NHCO2CH2Ph, and debenzylation.
IT 144675-54-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of intermediates for glycosylphosphatidylinositol anchors)
RN 144675-54-7 CAPLUS
CN D-myo-Inositol, 6-O-[(4-methoxyphenyl)methyl]-2,3,4,5-tetrakis-O-(phenylmethyl)-, (2R)-2,3-bis(tetradecyloxy)propyl hydrogen phosphate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 144675-53-6
CMF C73 H107 O12 P

L8 ANSWER 52 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



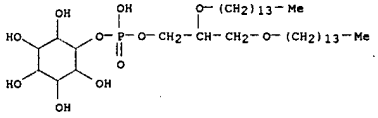
CM 2

CRN 121-44-8
CMF C6 H15 N

IT 144733-56-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for glycosylphosphatidylinositol anchors)
RN 144733-56-2 CAPLUS
CN D-myo-Inositol, 1-[(2R)-2,3-bis(tetradecyloxy)propyl hydrogen phosphate], compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 144485-59-6
CMF C37 H75 O11 P



CM 2

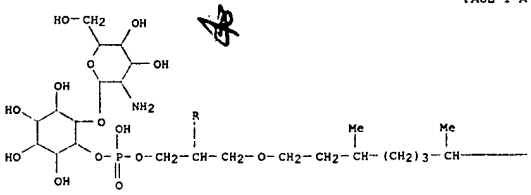
CRN 121-44-8
CMF C6 H15 N

L8 ANSWER 52 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

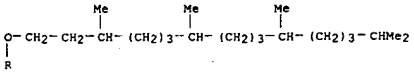
L8 ANSWER 53 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:486448 CAPLUS
DOCUMENT NUMBER: 117:86448
TITLE: Archaea contain a novel diether phosphoglycolipid with
a polar head group identical to the conserved core of eucaryal glycosyl phosphatidylinositol
AUTHOR(S): Nishihara, Masateru; Utagawa, Masami; Akutsu, Hideo; Koga, Yosuke
CORPORATE SOURCE: Sch. Med., Univ. Occup. Environ. Health, Kitakyushu, 807, Japan
SOURCE: Journal of Biological Chemistry (1992), 267(18), 12432-5
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of a major ether polar lipid of the methanogenic archaeon Methanosarcina barkeri was identified as glucosaminyl archaetidylinositol.
This lipid had archaeol (2,3-di-O-phytanyl-sn-glycerol) as a core lipid portion, and the polar head group consisted of 1 mol each of phosphate, myo-inositol, and D-glucosamine. The polar head group was identified by chemical degradation, phosphatidylinositol-specific phospholipase C treatment,
permethylation anal., and fast atom bombardment-mass spectrometry as glucosaminylinositol phosphate, which was linked to the glycerol backbone by a phosphodiester bond. The stereochem. configuration of the phospho-myo-inositol residue of glucosaminyl archaetidylinositol was determined
to be 1-D-myo-inositol 1-phosphate by measuring optical rotation of phospho-myo-inositol prepared by HNO2 deamination and alkaline hydrolysis from
the lipid. 1H-NMR of the intact lipid showed that GlcN was linked to C6 position of myo-inositol as an α-anomer. It is, finally, concluded that the complete structure of this lipid is 2,3-di-O-phytanyl-sn-glycero-
1-phospho-1'[6'-O-(2''-amino-2''-deoxy-α-D-glucopyranosyl)]-1'-D-myo-inositol. This lipid has a hybrid nature of an archaeal feature in alkyl glycerol diether core portion and a eucaryal feature in the polar head group identical to the conserved core structure (GlcNp(α1-6)-myo-inositol 1-phosphate) of glycosylated phosphatidylinositol, which serves as a membrane protein anchor in eucaryal cells.
IT 142978-49-2
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Methanosarcina barkeri)
RN 142978-49-2 CAPLUS
CN D-myo-Inositol, 6-O-(2-amino-2-deoxy-α-D-glucopyranosyl)-, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

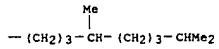
L8 ANSWER 53 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B





L8 ANSWER 54 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:243977 CAPLUS
DOCUMENT NUMBER: 114:243977
TITLE: Hydroxyarchaetidylserine and hydroxyarchaetidyl-myo-inositol in Methanosarcina barkeri: polar lipids with a new ether core portion
AUTHOR(S): Nishihara, Masateru; Koga, Yosuke
CORPORATE SOURCE: Dep. Chem., Univ. Occup. and Environ. Health, Kitakyushu, 807, Japan
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (1991), 1082(2), 211-17
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English

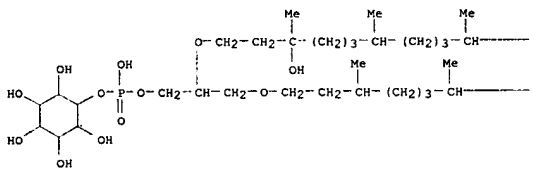
AB Lipids of the methanogenic archaebacterium M. barkeri were analyzed. The lipid content was 5.4% of dry cell and polar lipids comprised 87% of the total lipid. Polar lipids were separated into 14 spots by two-dimensional thin-layer chromatog. These were 6 phospholipids, 7 aminophospholipids and 1 glycolipid, of which 2 phospholipids and 2 aminophospholipids were major constituents. After removal of polar head groups from total lipids, 2 kinds of glycerol diether core lipids were found. One was 2,3-di-O-phytanyl-sn-glycerol (archaeol) and the other 2-O-(3'-hydroxy-3',7',11',15'-tetramethyl)hexadecyl-3-O-phytanyl-sn-glycerol (hydroxyarchaeol). Those structures were identified on the basis of chemical anal., fast atom bombardment-mass spectrometry, gas-liquid chromatog.-mass spectrometry and 1H- and 13C-NMR spectrometry. The latter was a new core lipid which was different from hydroxyarchaeol of Methanothrix concilii. The hydroxyarchaeol core lipid comprised 60% of polar lipid in M. barkeri. The structures of core lipids are quite different from those previously reported for M. barkeri lipids. The structures of 2 major polar lipids, both of which had hydroxyarchaeol as core portions, were elucidated. These lipids were 2-O-(3'-hydroxy)phytanyl-3-O-phytanyl-sn-glycero-1-phosphoserine (hydroxyarchaetidylserine) and 2-O-(3'-hydroxy)phytanyl-3-O-phytanyl-sn-glycero-1-phospho-myo-inositol (hydroxyarchaetidyl-myo-inositol). Archaetidylserine and archaetidylinositol, which had the usual archaeol core portion, were also present as minor polar lipids.

IT 134067-43-9
RL: BIOL (Biological study)
(from Methanosarcina barkeri, structure of)

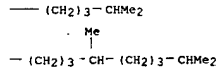
RN 134067-43-9 CAPLUS
CN D-myo-Inositol, 1-[(2S)-2-[[(7R,11R)-3-hydroxy-3,7,11,15-tetramethylhexadecyl]oxy]-3-[[(3R,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L8 ANSWER 54 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



L8 ANSWER 55 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:591094 CAPLUS
DOCUMENT NUMBER: 111:191094
TITLE: Complex lipids of Pyrococcus and AN1, thermophilic members of archaebacteria belonging to Thermococcales
AUTHOR(S): Lanzotti, Virginia; Trincone, Antonio; Nicolaus, Barbara; Zillig, Wolfram; De Rosa, Mario; Gambacorta, Agata
CORPORATE SOURCE: Ist. Chim. Mol. Interesse Biol., Cons. Naz. Ric., Naples, 80072, Italy
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (1989), 1004(1), 44-8
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English

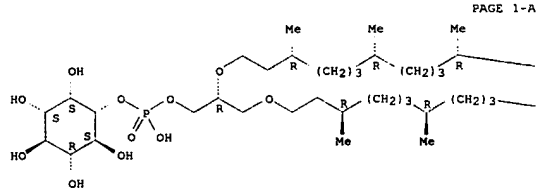
AB The lipid composition of two archaebacteria belonging to Thermococcales has been examined The major complex lipid present in the Pyrococcus genus is 2,3-di-O-phytanyl-sn-glycero-1-phosphoryl-1'-myo-L-inositol (90% of total lipids). In the AN1 isolate, this lipid (40% of total lipids) and a novel 2,3-di-O-phytanyl-sn-glycero-1-(α-D-glucopyranosyl 3-phosphate) (45%) were identified.

IT 123287-25-2
RL: PROC (Process)
(from Pyrococcus, characterization of)

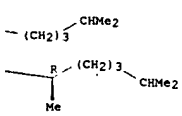
RN 123287-25-2 CAPLUS
CN D-myo-Inositol, 3-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate], stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



PAGE 1-B

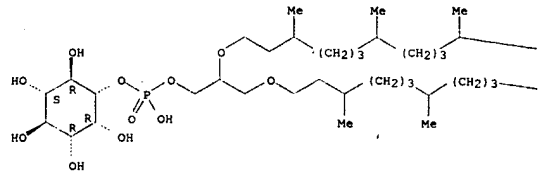


L8 ANSWER 55 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

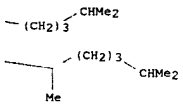
L8 ANSWER 56 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:474505 CAPLUS
DOCUMENT NUMBER: 111:74505
TITLE: Heptads of polar ether lipids of an archaebacterium, Methanobacterium thermoautotrophicum: structure and biosynthetic relationship [Erratum to document cited in CA110(5):36508a]
AUTHOR(S): Nishihara, Masateru; Morii, Hiroyuki; Koga, Yosuke
CORPORATE SOURCE: Dep. Chem., Univ. Occup. Environ. Health, Kitakyushu, 807, Japan
SOURCE: Biochemistry (1989), 28(13), 5702
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An error in the text has been corrected The error was not reflected in the abstract or the index entries.
IT 111955-11-4
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Methanobacterium thermoautotrophicum (Erratum))
RN 111955-11-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

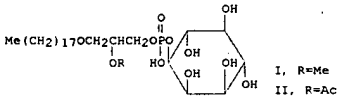


PAGE 1-B



L8 ANSWER 56 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L8 ANSWER 57 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:417222 CAPLUS
DOCUMENT NUMBER: 111:17222
TITLE: Synthesis and biological evaluation of ether-linked derivatives of phosphatidylinositol
AUTHOR(S): Ishaq, Khalid S.; Capobianco, Maria; Piantadosi, Claude; Noseda, Alessandro; Daniel, Larry W.; Modest, Edward J.
CORPORATE SOURCE: Sch. Pharm., Univ. North Carolina, Chapel Hill, NC, 27599, USA
SOURCE: Pharmaceutical Research (1989), 6(3), 216-24
CODEN: PHREEB; ISSN: 0724-8741
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

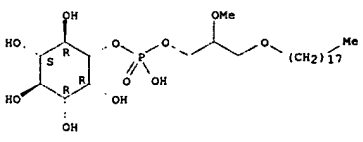


I, R=Me
II, R=Ac

AB The synthesis of two novel glycero-3-phosphoinositol ether lipid analogs, racemic-1-O-octadecyl-2-O-methylglycero-3-phospho-myo-inositol (I) (an ether lipid analog of racemic-1-O-octadecyl-2-O-methylglycero-3-phosphocholine; ET-18-OMe) and racemic-1-O-octadecyl-2-O-acetylglycero-3-phospho-myo-inositol (II) (an ether lipid analog of platelet-activating factor), is described. The two target compds. and the synthetic intermediates were evaluated for inhibition of HL60, BG1, and BG3 human malignant cells in vitro and inhibition of protein kinase C. Tumor inhibitory activity was found for I and II in all systems but not for their synthetic intermediates. However, I and II as well as some synthetic intermediates exhibited protein kinase C inhibitory activity.
IT 112924-43-3P 121244-57-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antitumor activity and protein kinase C inhibition by)
RN 112924-43-3 CAPLUS
CN myo-Inositol, 1-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

see 67

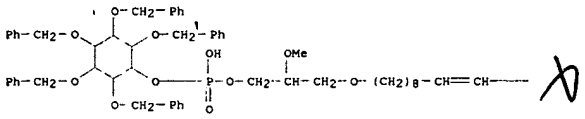
Relative stereochemistry.



RN 121244-57-3 CAPLUS

L8 ANSWER 57 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-methoxy-3-(9-octadecenyloxy)propyl hydrogen phosphate, (Z)- (9CI) (CA INDEX NAME)

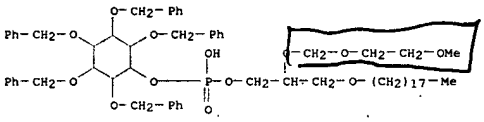
PAGE 1-A



PAGE 1-B

—(CH2)7—Me

IT 121244-54-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 121244-54-0 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-[(2-methoxyethoxy)methoxy]-3-(octadecyloxy)propyl hydrogen phosphate (9CI) (CA INDEX NAME)

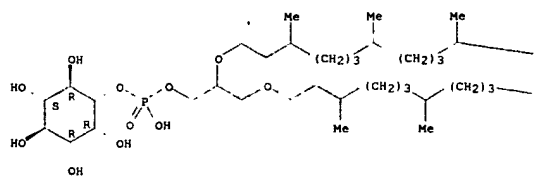


IT 121244-52-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 121244-52-8 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentakis-O-(phenylmethyl)-, 2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate (9CI) (CA INDEX NAME)

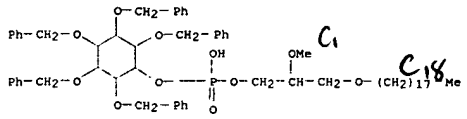
L8 ANSWER 58 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:131827 CAPLUS
DOCUMENT NUMBER: 110:131827
TITLE: Composition of polar lipids of Methanobrevibacter arboriphilicus and structure determination of the signature phosphoglycolipid of Methanobacteriaceae
AUTHOR(S): Morii, Hiroyuki; Nishihara, Masateru; Koga, Yosuke
CORPORATE SOURCE: Dep. Chem., Univ. Occup. Environ. Health Japan, Kitakyushu, 807, Japan
SOURCE: Agricultural and Biological Chemistry (1988), 52(12), 3149-56
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Total lipid was extracted effectively by the acidified Blight and Dyer solvent system from Methanobrevibacter arboriphilicus A2 cells. The lipid content was 5.8% of dry cell weight Cell disruption was required for the maximum yield of lipid from the cells. Eighteen polar lipids were detected and their composition was measured. Phosphoglycolipids from several species of Methanobacteriaceae which had the similar mobilities on thin-layer chromatograms were suggested as the common lipid of the family. The phosphoglycolipid (PGL1, 30%) from M. arboriphilicus was identified as gentiobiosyl caldarchaetidylinositol, which was identical to PGL1 of Methanobacterium thermautotrophicum. This confirmed that the lipid could be designated as the signature lipid of the family. The structure of the other major polar lipids were also identified as follows: gentiobiosyl caldarchaeol (GL1a, 9.9%), gentiobiosyl archaeol (GL1b, 12.6%), caldarchaetidylinositol (PL2a, 10.6%) and archaetidylinositol (PL2b, 3.1%).
IT 111955-11-4, Archaetidylinositol
RL: BIOL (Biological study)
(of Methanobrevibacter arboriphilicus, structure of)
RN 111955-11-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 57 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



$R_{2-6} = OCH_2Ph$

$R_{2-6} = O-CH_2-Ph$ (C7)

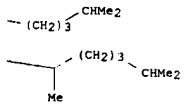
O-alkyl-aryl

$R_1 = C_{18}$

$R_7 =$

L8 ANSWER 58 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

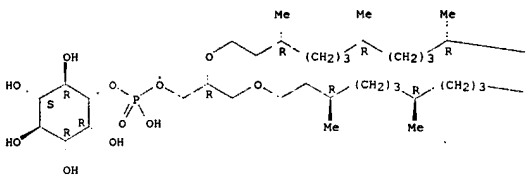
PAGE 1-B



L8 ANSWER 59 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:91715 CAPLUS
DOCUMENT NUMBER: 110:91715
TITLE: Structure of the major polar lipids isolated from the aceticlastic methanogen, Methanothrix concilii GP6
AUTHOR(S): Ferrante, Giulio; Ekiel, Irena; Patel, Girishchandra B.; Sprott, G. Dennis
CORPORATE SOURCE: Div. Biol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A OR6, Can.
SOURCE: Biochimica et Biophysica Acta, Lipids and Lipid Metabolism (1988), 963(2), 162-72
CODEN: BBLLA6; ISSN: 0005-2760
DOCUMENT TYPE: Journal
LANGUAGE: English
AB About 10% of the cell dry weight of the aceticlastic methanogen, M. concilii, was found to be lipid, consisting of 93% polar and 7% neutral lipids, resp. Several minor phospholipids and glycolipids were detected; however, the major lipid components, a phospholipid, and two glycolipids, accounted for approx. 84% of the total polar fraction. The three major polar lipids were identified as: (1) phospholipid; 2,3-di-O-phytanyl-sn-glycero-1-phosphoryl-1'-myo-L-inositol; (2) glycolopid-1; 2-O-phytanyl-3-O-[3'-hydroxy-3',7',11',15'-tetramethyl]hexadecyl-1-O-[β-D-galactopyranosyl-(1→6)-β-D-galactopyranosyl]-sn-glycerol; and (3) glycolipid-2; 2,3-diO-phytanyl-1-O-(α-D-mannopyran osyl-(1→3)-β-D-galactrpyranosyl]-sn-glycerol.
IT 109193-82-0
RL: BIOL (Biological study)
(from Methanothrix concilii, structure of)
RN 109193-82-0 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate], stereoisomer (9CI) (CA INDEX NAME)

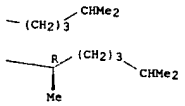
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 59 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B

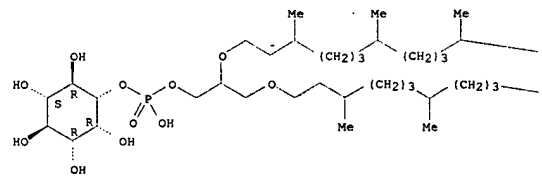


L8 ANSWER 60 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:36508 CAPLUS
DOCUMENT NUMBER: 110:36508
TITLE: Heptads of polar ether lipids of an archaebacterium, Methanobacterium thermoautotrophicum: structure and biosynthetic relationship
AUTHOR(S): Nishihara, Masateru; Morii, Hiroyuki; Koga, Yosuke
CORPORATE SOURCE: Dep. Chem., Univ. Occup. Environ. Health, Kitakyushu, 807, Japan
SOURCE: Biochemistry (1989), 28(1), 95-102
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structures of the 8 major polar lipids of M. thermoautotrophicum were determined They were a diether glycolipid (gentiobiosylarchaeol) and serine-, inositol-, and ethanolamine-containing diether and tetraether types of phospholipids and phosphoglycolipids [archaetidyl-L-serine, caldarchaetidyl-L-serine, gentiobiosylcaldarchaetidyl-L-serine, D-1-archaetidyl-myo-inositol, D-1-caldarchaetidyl-myo-inositol, D-1-(gentioibiosylcaldarchaetidyl)-myo-inositol, archaetidylethanolamine]. In combination with 2 neutral lipids and 3 polar lipids that have been already described, the 13 lipids were proposed to be classified in 3 groups, i.e., 3 heptads, each of which was constituted by diether and tetraether types of neutral lipids, glycolipids, and phospholipids, and a tetraether phosphoglycolipid. The heptad concept implied the biosynthetic relationship between diether and tetraether lipids which was supported by in vivo kinetic expts. When growing cells were pulse labeled with [32P]orthophosphate, there was a lag of 15-90 min between the rapid incorporation of label into diether polar lipids and that of label into the corresponding tetraether polar lipids. The lag times and rates of incorporation of 32P into tetraether phospholipids and their resp. diglucosyl derivs. (phosphoglycolipids) were almost identical. In a pulse-chase experiment with [32P]Pi, rapid turnover of the 3 diether lipids other than archaetidylethanolamine was observed At the same time radioactivity was incorporated into gentibiosylcaldarchaetidylinositol and other tetraether polar lipids. These results are consistent with a model which postulates that head-to-head condensation of phytanyl chains of 2 diether polar lipids occurs to yield tetraether polar lipids.
IT 111955-11-4
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Methanobacterium thermoautotrophicum)
RN 111955-11-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

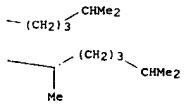
Absolute stereochemistry.

L8 ANSWER 60 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

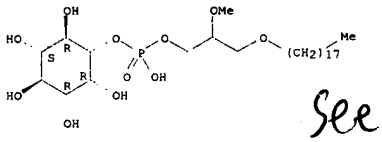


PAGE 1-B



L8 ANSWER 61 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:87587 CAPLUS
DOCUMENT NUMBER: 108:87587
TITLE: Neoplastic cell inhibition with new ether lipid analogs
AUTHOR(S): Noseda, Alessandro; Berens, Michael E.; Piantadosi, Claude; Modest, Edward J.
CORPORATE SOURCE: Bowman Gray Sch. Med., Wake Forest Univ., Winston-Salem, NC, 27103, USA
SOURCE: Lipids (1987), 22(11), 878-83
CODEN: LPDSAP; ISSN: 0024-4201
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bioactive phospholipid analogs of platelet-activating factor (PAF) represent a new approach to cancer chemotherapy. Various modifications of the basic structure of PAF lead to different ether lipid (EL) analogs. Data from the evaluation of thioalkyl and amidoalkyl glycerophosphocholine and of glycerophosphoinositol EL analogs against different exptl. tumors in vitro (HL60 and K562 human leukemia cells, BG1 and BG3 ovarian adenocarcinomas) are presented. Exclusion of trypan blue after short exposure to the drugs determined cytotoxicity, and a soft agarose clonogenic assay measured the ability of the analogs to inhibit tumor cell proliferation. The thioalkyl EL are very active against the cell lines using both end points, and the amidoalkyl EL showed efficacy against the leukemic cell lines, whereas the phosphoinositol EL are active only at high concns. Combined use of EL analogs, which are membrane-interactive, with classical DNA-interactive chemotherapeutic drugs revealed that the combinations have additive antiproliferative effects. These results are promising leads in the development of the anticancer potential of ether lipid analogs. Structure activity relationship is discussed.
IT 112924-43-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(neoplasm inhibition by)
RN 112924-43-3 CAPLUS
CN myo-Inositol, 1-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Relative stereochemistry.



claim 3

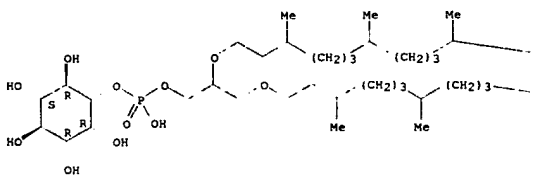
See 67

L8 ANSWER 61 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L8 ANSWER 62 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:18891 CAPLUS
DOCUMENT NUMBER: 108:18891
TITLE: Distribution of a diphytanyl ether analog of phosphatidylserine and an ethanolamine-containing tetraether lipid in methanogenic bacteria
AUTHOR(S): Koga, Yosuke; Oga, Mami; Nishihara, Masateru; Morii, Hiroyuki
CORPORATE SOURCE: Dep. Chem., Univ. Occup. Environ. Health, Kitakyushu, 807, Japan
SOURCE: Systematic and Applied Microbiology (1987), 9(3), 176-82
CODEN: SAMIDF; ISSN: 0723-2020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Aminolipids were found to be widely distributed in methanogens. Some of them were major components of the polar lipids. The distribution of two aminolipids, a diether analog of phosphatidylserine and a phosphoethanolamine derivative of dibiphytanyl diglycerol tetraether, was studied using TLC. In addition to the simple comparison of TLC patterns, the introduction of radiolabeled internal stds. greatly improved the reliability of TLC anal. of lipids. A ninhydrin-pos. spot which cochromatographed with the 32P-labeled diether analog of phosphatidylserine occurred as a major constituent in the total lipid in Methanobacteriaceae, but was absent in Methanomicrobiaceae and Methanosarcinaceae. Using the same method, the ethanolamine-containing tetraether phospholipid was found only in the genera Methanobacterium and Methanosarcina. A highly polar phosphoglycolipid was found only in Methanobacteriaceae. An aminolipid which migrated on TLC between phosphatidylserine and phosphatidylethanolamine was confined to Methanomicrobiaceae. It is suggested that the occurrence of these polar lipids be used for the grouping of methanogens at the family level.
IT 111955-11-4
RL: BIOL (Biological study)
(of methanogenic bacteria, taxonomy in relation to)
RN 111955-11-4 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

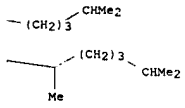
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 62 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



L8 ANSWER 63 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:436269 CAPLUS
DOCUMENT NUMBER: 107:36269
TITLE: Lipids of Thermococcus celer, a sulfur-reducing archaebacterium: structure and biosynthesis
AUTHOR(S): De Rosa, Mario; Gambacorta, Agata; Trincone, Antonio; Basso, Annalisa; Zillig, Wolfram; Holz, Ingelore
CORPORATE SOURCE: Ist. Chim. Mol. Interesse Biol., Naples, Italy
SOURCE: Systematic and Applied Microbiology (1987), 9(1-2), 1-5
CODEN: SAMIDF; ISSN: 0723-2020
DOCUMENT TYPE: Journal
LANGUAGE: English

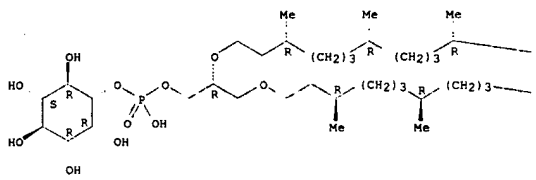
AB The lipids of T. celer, an extremely thermophilic anaerobic sulfur-respiring archaebacterium, are characterized. On the basis of spectroscopic (1H and 13C-NMR), chromatog., and degradation studies, the most abundant polar lipid (about 80% of total lipid extract) was identified as 2,3-di-O-phytanyl-sn-glycerol ester of phosphatidyl-myo-inositol. Its biosynthesis from acetate was shown by the incorporation of 14C labeled acetate.

IT 109193-82-0
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Thermococcus celer)

RN 109193-82-0 CAPLUS
CN D-myo-Inositol, 1-[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propyl hydrogen phosphate], stereoisomer (9CI) (CA INDEX NAME)

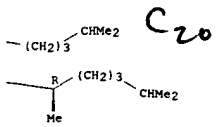
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 63 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



L8 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:572785 CAPLUS
DOCUMENT NUMBER: 105:172785
TITLE: Glycerol ether phosphatides and their use
INVENTOR(S): Breuninger, Manfred; Schmidt, Dieter
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 154977	A2	19850918	EP 1985-102830	19850312
EP 154977	A3	19860219		
EP 154977	B1	19890517		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CA 1264162	A1	19900102	CA 1985-475022	19850225
IL 74540	A1	19890228	IL 1985-74540	19850307
ZA 8501774	A	19861029	ZA 1985-1774	19850308
US 4694084	A	19870915	US 1985-709871	19850308
AU 8539710	A1	19850919	AU 1985-39710	19850311
AU 574440	B2	19880707		
FI 8500972	A	19850916	FI 1985-972	19850312
FI 78299	B	19890331		
FI 78299	C	19890710		
AT 43131	E	19890615	AT 1985-102830	19850312
HU 36824	A2	19851028	HU 1985-923	19850313
HU 195828	B	19880728		
JP 60215693	A2	19851029	JP 1985-48452	19850313
DK 8501179	A	19850916	DK 1985-1179	19850314
NO 8501006	A	19850916	NO 1985-1006	19850314
ES 541242	A1	19860416	ES 1985-541242	19850314
CN 85103123	A	19861022	CN 1985-103123	19850423
CN 1009931	B	19901010		
ES 550920	A1	19870216	ES 1986-550920	19860116

PRIORITY APPLN. INFO.:
CH 1984-1287 A 19840315
CH 1985-491 A 19850204
EP 1985-102830 A 19850312

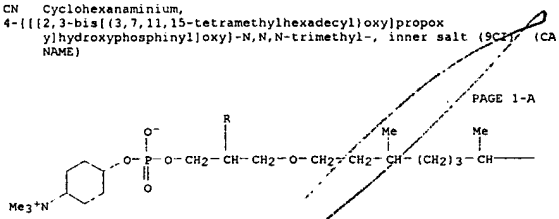
AB The title compds., useful for preparation of colloidal solns., e.g., liposome and mixed micelle solns. for drug solubilization, were prepared Thus, 2.09 mmol (RS)-2,3-bis[[(3RS,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propano l was added to a mixture of 8.4 mmol Et3N, CHCl3, and POCl3 at -78°, the resulting mixture cooled for 1 h and then warmed to 0°, 3.2 mmol choline tosylate in pyridine added over 30 min, and the resulting mixture stirred at room temperature for a few hours to give O-[[(RS)-2,3-bis[[(3RS,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propyl]hydroxyphosphi nyl]choline hydroxide (inner salt). A mixture of 1.0 g [4-[[[(RS)-2,3-bis[[(3RS,7R,11R)-3,7,11,15-tetramethylhexadecyl]oxy]propoxy]hydroxyphosph inyl]oxy]butyl]trimethylammonium hydroxide (inner salt), 2.4 g sucrose, and 7.5 mL H2O was stirred for 1 h, the milky dispersion was sonicated for 20 min, and the resulting weakly opalescent liposome soln. was centrifuged, filtered, placed in ampuls, and heated at 120° for 20 min to give a sterilized multilamellar liposome soln.

L8 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

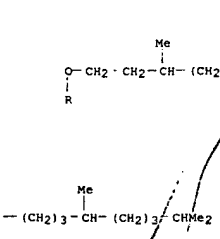
IT 103023-21-8P 103023-22-9P 103023-23-0P
103023-24-1P 103023-25-2P 103023-26-3P
103023-27-4P 103023-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for liposome)

RN 103023-21-8 CAPLUS
CN Cyclohexanaminium, 4-[[[2,3-bis[(3,7,11,15-tetramethylhexadecyl)oxy]propox y]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



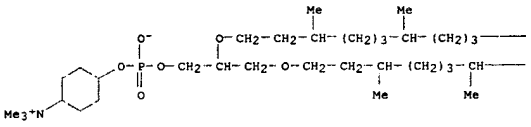
PAGE 1-B



RN 103023-22-9 CAPLUS
CN Cyclohexanaminium, 4-[[[2,3-bis[(3,7,11-trimethyldodecyl)oxy]propoxy]hydro xyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

L8 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



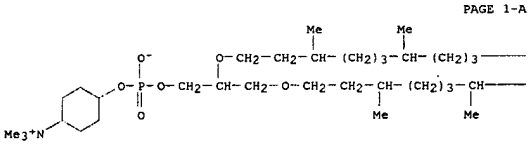
PAGE 1-B

— $CHMe_2$

— $(CH_2)_3-CHMe_2$

RN 103023-23-0 CAPLUS
CN Cyclohexanaminium, 4-[[hydroxy[3-[(3,7,11,15-tetramethylhexadecyl)oxy]-2-[(3,7,11-trimethyldodecyl)oxy]propoxy]phosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

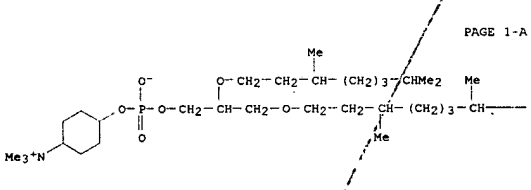
— $CHMe_2$ Me

— $(CH_2)_3-CH-(CH_2)_3-CHMe_2$

RN 103023-24-1 CAPLUS
CN Cyclohexanaminium, 4-[[[2-[(3,7-dimethyloctyl)oxy]-3-[(3,7,11,15-tetramethylhexadecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

L8 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
inner salt (9CI) (CA INDEX NAME)

PAGE 1-A

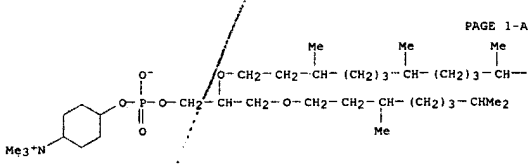


PAGE 1-B

— $(CH_2)_3-CHMe_2$

RN 103023-27-4 CAPLUS
CN Cyclohexanaminium, 4-[[[3-[(3,7-dimethyloctyl)oxy]-2-[(3,7,11,15-tetramethylhexadecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



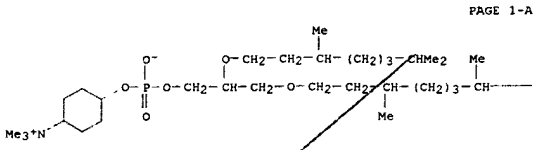
PAGE 1-B

— $(CH_2)_3-CHMe_2$

RN 103023-28-5 CAPLUS
CN Cyclohexanaminium, 4-[[[3-[(3,7-dimethyloctyl)oxy]-2-[(3,7,11-trimethyldodecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

L8 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

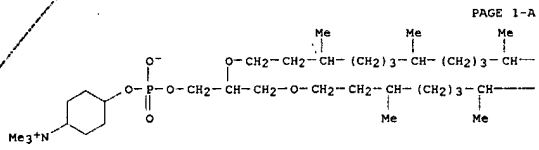


PAGE 1-B

— $(CH_2)_3-CH-(CH_2)_3-CHMe_2$
Me

RN 103023-25-2 CAPLUS
CN Cyclohexanaminium, 4-[[hydroxy[2-[(3,7,11,15-tetramethylhexadecyl)oxy]-3-[(3,7,11-trimethyldodecyl)oxy]propoxy]phosphinyl]oxy]-N,N,N-trimethyl-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

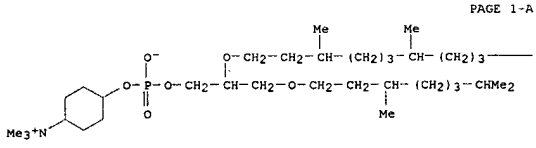
——— $(CH_2)_3-CHMe_2$

— $(CH_2)_3-CHMe_2$

RN 103023-26-3 CAPLUS
CN Cyclohexanaminium, 4-[[[2-[(3,7-dimethyloctyl)oxy]-3-[(3,7,11-trimethyldodecyl)oxy]propoxy]hydroxyphosphinyl]oxy]-N,N,N-trimethyl-,

L8 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



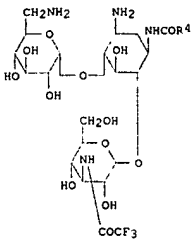
PAGE 1-B

— $CHMe_2$

L8 ANSWER 65 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:39731 CAPLUS
DOCUMENT NUMBER: 104:39731
TITLE: Pharmaceutical emulsions
INVENTOR(S): Ueda, Yoshio; Ito, Toshio; Honbo, Toshiyasu; Yamamoto, Takao
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60166610	A2	19850829	JP 1984-24047	19840209
PRIORITY APPLN. INFO.:			JP 1984-24047	19840209

GI



I

AB A pharmaceutical emulsion contains a glycerol derivative R1(CO)nOCH2CH(OR2)CH2OP(O)(Y)O(CH2CH2)mR3 (R1 = alkyl; R2 = H, alkyl; R3 = inositol residue, N-containing cyclic ring, trimethylammonio; Y = OH, oxide; m, n = 0, 1) or its salts, or the kanamycin derivative I (R4 = alkyl) or its salts with addition of >10 weight/volume% oils to prevent or reduce the hemolytic activity of the active ingredients. Thus, soybean oil 2.0 and egg yolk lecithin 7.5 were mixed, heated at 65-75° and cooled to room temperature, and to this was added 1.0 g I (R4 = nonadecyl), 2.5 g glycerol and H2O (to

Kokusho
US 4783402

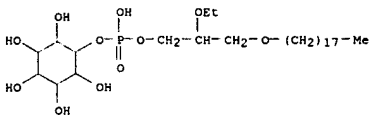
L8 ANSWER 66 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:77260 CAPLUS
DOCUMENT NUMBER: 102:77260
TITLE: Primary or secondary alcohol derivatives of phospholipids produced by the enzymic technique
INVENTOR(S): Kokusho, Yoshitaka; Kato, Shigeaki; Machida, Haruo
PATENT ASSIGNEE(S): Meito Sangyo Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 80 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 122151	A2	19841017	EP 1984-302444	19840410
EP 122151	A3	19860326		
EP 122151	B1	19890215		
R: CH, DE, FR, GB, IT, LI, NL				
JP 59187786	A2	19841024	JP 1983-63305	19830411
JP 02008716	B4	19900226		
JP 60041494	A2	19850305	JP 1983-63304	19830411
JP 02007633	B4	19900220		
US 4783402	A	19881108	US 1984-598697	19840410
PRIORITY APPLN. INFO.:			JP 1983-63304 A	19830411
			JP 1983-63305 A	19830411

OTHER SOURCE(S): MARPAT 102:77260
AB Primary and secondary alc. derivs. of phospholipids are produced by reacting the alc. with a lecithin, catalyzed by phospholipase (9013-93-8) DM from Nocardiopsis or Actinomadura. Thus, 400 mg β-γ-dihexadecyl-L-α-lecithin [36314-47-3] was emulsified in 1 mL ether and 10 mL H2O. Then, 2 mL emulsion was mixed with 2 mL pH 5.7 0.4M acetate buffer, 1 mL 0.1M CaCl2, 2 mL 10% solution of thiamin [59-43-8] HCl in ether, and 2 mL aqueous solution of phospholipase DM (2.5 units/mL) and let stand at 37° for 3 h. The yield of the thiamin derivative of 1,2-dihexadecyl-sn-glycerol 3-phosphoric acid [94475-74-8] was 30 mg.
IT 94456-72-1P 94456-73-2P
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, from lecithin and alc., enzymic)
RN 94456-72-1 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] monocyclohexyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

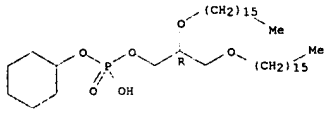
L8 ANSWER 65 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
20 mL). The mixt. was sonicated to give an emulsion.
IT 99783-02-5
RL: BIOL (Biological study)
(pharmaceutical emulsion containing soybean oil and, hemolytic activity prevention in relation to)
RN 99783-02-5 CAPLUS
CN myo-Inositol, 2-[2-ethoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI)
(CA INDEX NAME)



✓ see 62

$R_2-R_6 = H$, $X=O$, $Y=O$, $A = \overset{O}{\overset{\|}{P}}OH$

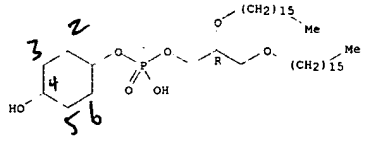
L8 ANSWER 66 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



✗ R1 = AK, R1 = AK

RN 94456-73-2 CAPLUS
CN Phosphoric acid, mono[2,3-bis(hexadecyloxy)propyl] mono(4-hydroxycyclohexyl) ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



$R_1 = C_{16}$, $R_2 = C_{16}$

$R_{2,3,5,6} = H$, $R_4 = OH$

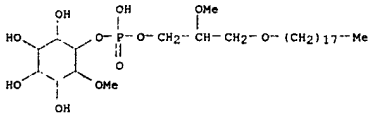
✗ 1, 2, 5, 6-8, 10, 20, 21, 23, 24, 25, 27,

L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:423888 CAPLUS
DOCUMENT NUMBER: 101:23888
TITLE: Phospholipid derivatives and their pharmaceutical compositions
INVENTOR(S): Tsutomu, Teraji; Eishiro, Todo; Norihiko, Shimazaki; Teruo, Oku; Takayuki, Namiki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 51 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

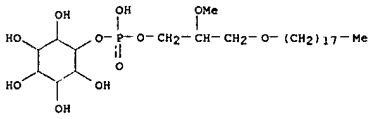
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 100499	A2	19840215	EP 1983-107236	19830723
EP 100499	A3	19850612		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4585762	A	19860429	US 1983-513451	19830713
DK 8303473	A	19840131	DK 1983-3473	19830728
JP 59042394	A2	19840308	JP 1983-139709	19830729
ES 524610	A1	19841201	ES 1983-524610	19830729
ES 530669	A1	19850501	ES 1984-530669	19840315
ES 530668	A1	19850701	ES 1984-530668	19840315
PRIORITY APPLN. INFO.:			GB 1982-22020 A	19820730

OTHER SOURCE(S): MARPAT 101:23888
AB RCH2(CHR1)nCH2OP(O)R2R3 [R = alkyl, alkoxy, alkylthio, alkylsulfonyl; R1 = H, OH, alkoxy, alkanoyloxy, alkylcarbamoyloxy; n = 0, 1; R2 = (un)protected OH; R3 = alkoxy, alacyclic oxy group with ≥2 (un)protected OH groups], or their pharmaceutically acceptable salts, were prepared as antitumor agents. Thus, DL-2-methoxyoctadecyl 2-(1,3,4,5,6-penta-O-acetyl-DL-myo-inositylˆ) Ph phosphate was obtained from Ag 2-(1,3,4,5,6-penta-O-acetyl-DL-myo-inositylˆ) Ph phosphate and DL-2-methoxyoctadecyl iodide. The product was hydrogenolized, then treated with ion-exchange resin (Dowex 50) to give DL-2-methoxyoctadecyl 2-(DL-myo-inositylˆ) phosphate (I). I was a more effective antitumor agent against fibrosarcoma Meth A in female mice than was 1-O-octadecyl-2-O-methylglycerol-3-phosphorylcholine.
IT 90339-54-1P 90366-37-3P 90366-41-9P
99783-02-5P 112924-43-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)
RN 90339-54-1 CAPLUS
CN myo-Inositol, 1-O-methyl-, 2-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

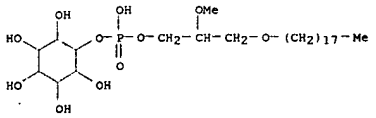


RN 90366-37-3 CAPLUS
CN chiro-Inositol, 2-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



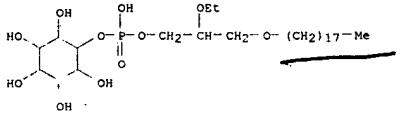
X=O
Y=O

RN 90366-41-9 CAPLUS
CN chiro-Inositol, 1-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



R_2 = Me (C_1)
R_1 = C_{18}

RN 99783-02-5 CAPLUS
CN myo-Inositol, 2-[2-ethoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI)
(CA INDEX NAME)



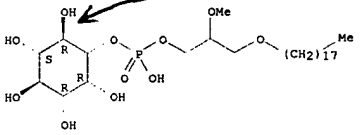
R_1 = C_{18}

1,3,7,

L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

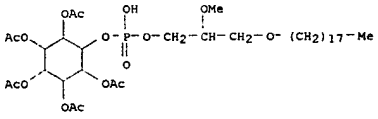
RN 112924-43-3 CAPLUS
CN myo-Inositol, 1-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Relative stereochemistry.



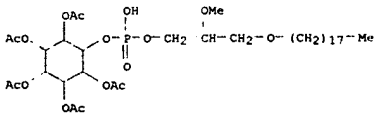
(1a) claim 3
1-3, 5-13
28, 37

IT 90366-44-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
RN 90366-44-2 CAPLUS
CN myo-Inositol, 1,2,4,5,6-pentaacetate 3-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



X

IT 90339-15-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 90339-15-4 CAPLUS
CN myo-Inositol, 1,3,4,5,6-pentaacetate 2-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate], monopotassium salt (9CI) (CA INDEX NAME)

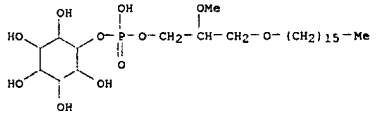


X

● K

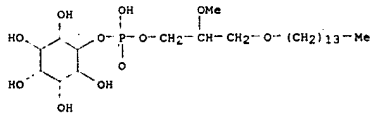
L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 90339-22-3P 90339-24-5P 90339-37-0P
90339-45-0P 90410-02-9P 90410-05-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ion-exchange reaction of)
RN 90339-22-3 CAPLUS
CN myo-Inositol, 2-[3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)



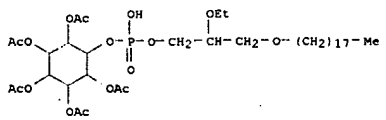
● Na

RN 90339-24-5 CAPLUS
CN myo-Inositol, 2-[2-methoxy-3-(tetradecyloxy)propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)



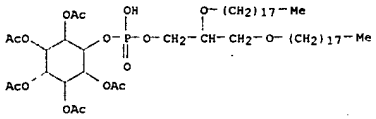
● Na

RN 90339-37-0 CAPLUS
CN myo-Inositol, 1,3,4,5,6-pentaacetate 2-[2-ethoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

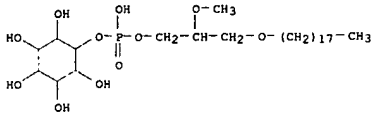


X

L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 90339-45-0 CAPLUS
CN myo-Inositol, 1,3,4,5,6-pentaacetate 2-[2,3-bis(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

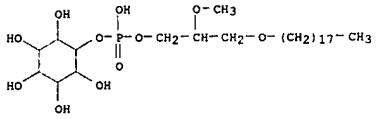


RN 90410-02-9 CAPLUS
CN chiro-Inositol, 2-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)



● Na

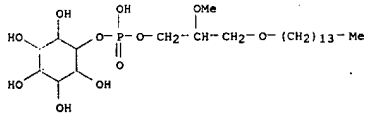
RN 90410-05-2 CAPLUS
CN chiro-Inositol, 1-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate], monosodium salt (9CI) (CA INDEX NAME)



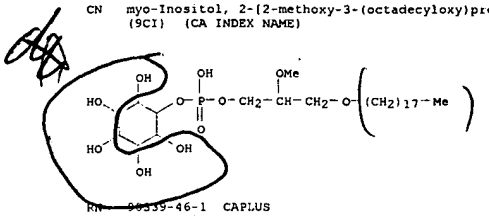
● Na

IT 90339-16-5P 90339-46-1P 90366-26-0P
90366-27-1P

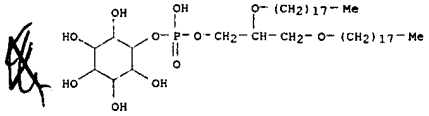
L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



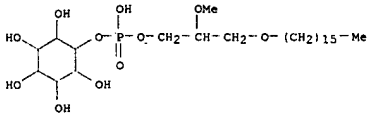
L8 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 90339-16-5 CAPLUS
CN myo-Inositol, 2-[2-methoxy-3-(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



RN 90339-46-1 CAPLUS
CN myo-Inositol, 2-[2,3-bis(octadecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

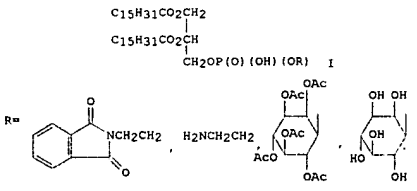


RN 90366-26-0 CAPLUS
CN myo-Inositol, 2-[3-(hexadecyloxy)-2-methoxypropyl hydrogen phosphate] (9CI) (CA INDEX NAME)

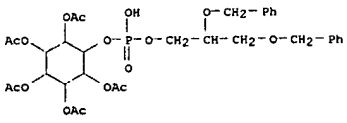


RN 90366-27-1 CAPLUS
CN myo-Inositol, 2-[2-methoxy-3-(tetradecyloxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)

L8 ANSWER 68 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:62556 CAPLUS
DOCUMENT NUMBER: 88:62556
TITLE: Studies on complex lipids. Synthesis of phosphatidylethanolamine and phosphatidylinositol by direct acylation of glycerolphosphoric acid esters by aliphatic acid anhydrides
AUTHOR(S): Sukhanov, V. A.; Sergovskaya, N. L.; Shvets, V. I.; Evstigneeva, R. P.
CORPORATE SOURCE: Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SOURCE: Zhurnal Obshchei Khimii (1977), 47(9), 2130-6
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



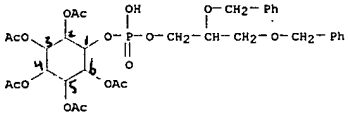
AB Glyceride phosphates I was obtained in 58-89% yields in 3 steps from 1,2-di-O-benzylglycerol by phosphorylation with (HO)2P(O)(OR), debenzylation, and esterification with palmitic acid. Similarly HOCH2CH(OH)CH2OP(O)(OH)OCH2CH(NHCO2CH2Ph)CO2CH2Ph was obtained in 76.7% from 1-O-benzylglycerol by acetylation, debenzylation, phosphorylation, saponification, and treatment with DL-serine.
IT 65391-08-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)
RN 65391-08-4 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentaacetate 1-[(2R)-2,3-bis(phenylmethoxy)propyl hydrogen phosphate] (9CI) (CA INDEX NAME)



L8 ANSWER 68 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L8 ANSWER 69 OF 69 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1977:171755 CAPLUS
DOCUMENT NUMBER: 86:171755
TITLE: Synthesis of phosphatidylethanolamine and phosphatidylinositol
AUTHOR(S): Sukhanov, V. A.; Sergovskaya, N. L.; Shvets, V. I.; Estigneeva, R. P.
CORPORATE SOURCE: USSR
SOURCE: Tr. Mosk. In-ta Tonkoi Khim. Tekhnol. (1975), (6), 76-8
From: Ref. Zh., Khim. 1976, Abstr. No. 24E125
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.
IT 62700-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 62700-92-9 CAPLUS
CN D-myo-Inositol, 2,3,4,5,6-pentaacetate 1-(2,3-bis(phenylmethoxy)propyl hydrogen phosphate) (9CI) (CA INDEX NAME)



X

R_{2-6} = OAc Not Claimed